## Second Edition



## Physical-Chemical Properties and Environmental Fate for Organic Chemicals

Volume I
Introduction and Hydrocarbons
Volume II
Halogenated Hydrocarbons

## Volume III <br> Oxygen Containing Compounds

Volume IV
Nitrogen and Sulfur Containing Compounds and Pesticides

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## Physical-Chemical

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Nitrogen and Sulfur Containing Compounds and Pesticides

Donald Mackay
Wan Ying Shiu
Kuo-Ching Ma
Sum Chi Lee

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## Preface

This handbook is a compilation of environmentally relevant physical-chemical data for similarly structured groups of chemical substances. These data control the fate of chemicals as they are transported and transformed in the multimedia environment of air, water, soils, sediments, and their resident biota. These fate processes determine the exposure experienced by humans and other organisms and ultimately the risk of adverse effects. The task of assessing chemical fate locally, regionally, and globally is complicated by the large (and increasing) number of chemicals of potential concern; by uncertainties in their physical-chemical properties; and by lack of knowledge of prevailing environmental conditions such as temperature, pH , and deposition rates of solid matter from the atmosphere to water, or from water to bottom sediments. Further, reported values of properties such as solubility are often in conflict. Some are measured accurately, some approximately, and some are estimated by various correlation schemes from molecular structures. In some cases, units or chemical identity are wrongly reported. The user of such data thus has the difficult task of selecting the "best" or "right" values. There is justifiable concern that the resulting deductions of environmental fate may be in substantial error. For example, the potential for evaporation may be greatly underestimated if an erroneously low vapor pressure is selected.

To assist the environmental scientist and engineer in such assessments, this handbook contains compilations of physical-chemical property data for over 1000 chemicals. It has long been recognized that within homologous series, properties vary systematically with molecular size, thus providing guidance about the properties of one substance from those of its homologs. Where practical, plots of these systematic property variations can be used to check the reported data and provide an opportunity for interpolation and even modest extrapolation to estimate unmeasured properties of other substances. Most handbooks treat chemicals only on an individual basis and do not contain this feature of chemical-to-chemical comparison, which can be valuable for identifying errors and estimating properties. This most recent edition includes about 1250 compounds and contains about 30 percent additional physical-chemical property data. There is a more complete coverage of PCBs, PCDDs, PCDFs, and other halogenated hydrocarbons, especially brominated and fluorinated substances that are of more recent environmental concern. Values of the physical-chemical properties are generally reported in the literature at a standard temperature of 20 or $25^{\circ} \mathrm{C}$. However, environmental temperatures vary considerably, and thus reliable data are required on the temperature dependence of these properties for fate calculations. A valuable enhancement to this edition is the inclusion of extensive measured temperature-dependent data for the first time. The data focus on water solubility, vapor pressure, and Henry's law constant but include octanol/water and octanol/air partition coefficients where available. They are provided in the form of data tables and correlation equations as well as graphs.

We also demonstrate in Chapter 1 how the data may be taken a stage further and used to estimate likely environmental partitioning tendencies, i.e., how the chemical is likely to become distributed between the various media that comprise our biosphere. The results are presented numerically and pictorially to provide a visual impression of likely environmental behavior. This will be of interest to those assessing environmental fate by confirming the general fate characteristics or behavior profile. It is, of course, only possible here to assess fate in a "typical" or "generic" or "evaluative" environment. No claim is made that a chemical will behave in this manner in all situations, but this assessment should reveal the broad characteristics of behavior. These evaluative fate assessments are generated using simple fugacity models that flow naturally from the compilations of data on physical-chemical properties of relevant chemicals. Illustrations of estimated environmental fate are given in Chapter 1 using Levels I, II, and III mass balance models. These and other models are available for downloading gratis from the website of the Canadian Environmental Modelling Centre at Trent University (www.trent.ca/cemc).

It is hoped that this new edition of the handbook will be of value to environmental scientists and engineers and to students and teachers of environmental science. Its aim is to contribute to better assessments of chemical fate in our multimedia environment by serving as a reference source for environmentally relevant physical-chemical property data of classes of chemicals and by illustrating the likely behavior of these chemicals as they migrate throughout our biosphere.

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## Biographies

Donald Mackay, born and educated in Scotland, received his degrees in Chemical Engineering from the University of Glasgow. After working in the petrochemical industry he joined the University of Toronto, where he taught for 28 years in the Department of Chemical Engineering and Applied Chemistry and in the Institute for Environmental Studies. In 1995 he moved to Trent University to found the Canadian Environmental Modelling Centre. Professor Mackay's primary research is the study of organic environmental contaminants, their properties, sources, fates, effects, and control, and particularly understanding and modeling their behavior with the aid of the fugacity concept. His work has focused especially on the Great Lakes Basin; on cold northern climates; and on modeling bioaccumulation and chemical fate at local, regional, continental and global scales.

His awards include the SETAC Founders Award, the Honda Prize for Eco-Technology, the Order of Ontario, and the Order of Canada. He has served on the editorial boards of several journals and is a member of SETAC, the American Chemical Society, and the International Association of Great Lakes Research.

Wan-Ying Shiu is a Senior Research Associate in the Department of Chemical Engineering and Applied Chemistry, and the Institute for Environmental Studies, University of Toronto. She received her Ph.D. in Physical Chemistry from the Department of Chemistry, University of Toronto, M.Sc. in Physical Chemistry from St. Francis Xavier University, and B.Sc. in Chemistry from Hong Kong Baptist College. Her research interest is in the area of physical-chemical properties and thermodynamics for organic chemicals of environmental concern.

Kuo-Ching Ma obtained his Ph.D. from Florida State University, M.Sc. from The University of Saskatchewan, and B.Sc. from The National Taiwan University, all in Physical Chemistry. After working many years in the aerospace, battery research, fine chemicals, and metal finishing industries in Canada as a Research Scientist, Technical Supervisor/ Director, he is now dedicating his time and interests to environmental research.

Sum Chi Lee received her B.A.Sc. and M.A.Sc. in Chemical Engineering from the University of Toronto. She has conducted environmental research at various government organizations and the University of Toronto. Her research activities have included establishing the physical-chemical properties of organochlorines and understanding the sources, trends, and behavior of persistent organic pollutants in the atmosphere of the Canadian Arctic.

Ms. Lee also possesses experience in technology commercialization. She was involved in the successful commercialization of a proprietary technology that transformed recycled material into environmentally sound products for the building material industry. She went on to pursue her MBA degree, which she earned from York University's Schulich School of Business. She continues her career, combining her engineering and business experiences with her interest in the environmental field.

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### 1.1 THE INCENTIVE

It is believed that there are some 50,000 to 100,000 chemicals currently being produced commercially in a range of quantities with approximately 1000 being added each year. Most are organic chemicals, and many are pesticides and biocides designed to modify the biotic environment. Of these, perhaps 1000 substances are of significant environmental concern because of their presence in detectable quantities in various components of the environment, their toxicity, their tendency to bioaccumulate, their persistence and their potential to be transported long distances. Some of these chemicals, including pesticides, are of such extreme environmental concern that international actions have been taken to ensure that all production and use should cease, i.e., as a global society we should elect not to synthesize or use these chemicals. They should be "sunsetted." PCBs, "dioxins" and DDT are examples. A second group consists of less toxic and persistent chemicals which are of concern because they are used or discharged in large quantities. They are, however, of sufficient value to society that their continued use is justified, but only under conditions in which we fully understand and control their sources, fate and the associated risk of adverse effects. This understanding is essential if society is to be assured that there is negligible risk of adverse ecological or human health effects. Other groups of more benign chemicals can presumably be treated with less rigor.

A key feature of this "cradle-to-grave" approach to chemical management is that society must improve its skills in assessing chemical fate in the environment. We must better understand where chemicals originate, how they migrate in, and between, the various media of air, water, soils, sediments and their biota which comprise our biosphere. We must understand how these chemicals are transformed by chemical and biochemical processes and, thus, how long they will persist in the environment. We must seek a fuller understanding of the effects that they will have on the multitude of interacting organisms that occupy these media, including ourselves.

It is now clear that the fate of chemicals in the environment is controlled by a combination of three groups of factors. First are the prevailing environmental conditions such as temperatures, flows and accumulations of air, water and solid matter and the composition of these media. Second are the properties of the chemicals which influence partitioning and reaction tendencies, i.e., the extent to which the chemical evaporates or associates with sediments, and how fast the chemical is eventually destroyed by conversion to other chemical species. Third are the patterns of use, into which compartments the substance is introduced, whether introduction is episodic or continuous and in the case of pesticides how and with which additives the active ingredient is applied.

In recent decades there has emerged a discipline within environmental science concerned with increasing our understanding of how chemicals behave in our multimedia environment. It has been termed environmental chemistry or "chemodynamics." Practitioners of this discipline include scientists and engineers, students and teachers who attempt to measure, assess and predict how this large number of chemicals will behave in laboratory, local, regional and global environments. These individuals need data on physical-chemical and reactivity properties, as well as information on how these properties translate into environmental fate. This handbook provides a compilation of such data and outlines how to use them to estimate the broad features of environmental fate. It does so for classes or groups of chemicals, instead of the usual approach of treating chemicals on an individual basis. This has the advantage that systematic variations in properties with molecular structure can be revealed and exploited to check reported values, interpolate and even extrapolate to other chemicals of similar structure.

With the advent of inexpensive and rapid computation there has been a remarkable growth of interest in this general area of quantitative structure-property relationships (QSPRs). The ultimate goal is to use information about chemical structure to deduce physical-chemical properties, environmental partitioning and reaction tendencies, and even uptake and effects on biota. The goal is far from being fully realized, but considerable progress has been made. In this series of handbooks we have adopted a simple and well-tried approach of using molecular structure to deduce a molar volume, which in turn is related to physical-chemical properties. In the case of pesticides, the application of QSPR approaches is complicated by the large number of chemical classes, the frequent complexity of molecules and the lack of experimental data. Where there is a sufficient number of substances in each class or homologous series QSPRs are presented, but in some cases there is a lack of data to justify them. QSPRs based on other more complex molecular descriptors are, of course, widely available, especially in the proceedings of the biennial QSAR conferences.

Regrettably, the scientific literature contains a great deal of conflicting data, with reported values often varying over several orders of magnitude. There are some good, but more not-so-good reasons for this lack of accuracy. Many of these properties are difficult to measure because they involve analyzing very low concentrations of 1 part in $10^{9}$ or $10^{12}$. For many purposes an approximate value is adequate. There may be a mistaken impression that if a vapor pressure is low, as is the case with DDT, it is not important. DDT evaporates appreciably from solution in water, despite its low vapor pressure, because of its low solubility in water. In some cases the units are reported incorrectly. There may be uncertainties about temperature or pH . In other cases the chemical is wrongly identified. Errors tend to be perpetuated
by repeated citation. The aim of this handbook is to assist the user to identify such problems, provide guidance when selecting appropriate values and where possible determine their temperature dependence.

The final aspect of chemical fate treated in this handbook is the depiction or illustration of likely chemical fate. This is done using multimedia "fugacity" models as described later in this chapter. The aim is to convey an impression of likely environmental partitioning and transformation characteristics, i.e., a "behavior profile." A fascinating feature of chemodynamics is that chemicals differ so greatly in their behavior. Some, such as chloroform, evaporate rapidly and are dissipated in the atmosphere. Others, such as DDT, partition into the organic matter of soils and sediments and the lipids of fish, birds and mammals. Phenols and carboxylic acids tend to remain in water where they may be subject to fairly rapid transformation processes such as hydrolysis, biodegradation and photolysis. By entering the physicalchemical data into a model of chemical fate in a generic or evaluative environment, it is possible to estimate the likely general features of the chemical's behavior and fate. The output of these calculations can be presented numerically and pictorially.

In summary, the aim of this series of handbooks is to provide a useful reference work for those concerned with the assessment of the fate of existing and new chemicals in the environment.

### 1.2 PHYSICAL-CHEMICAL PROPERTIES

### 1.2.1 The Key Physical-Chemical Properties

In this section we describe the key physical-chemical properties and discuss how they may be used to calculate partition coefficients for inclusion in mass balance models. Situations in which data require careful evaluation and use are discussed.

The major differences between behavior profiles of organic chemicals in the environment are attributable to their physical-chemical properties. The key properties are recognized as solubility in water, vapor pressure, the three partition coefficients between air, water and octanol, dissociation constant in water (when relevant) and susceptibility to degradation or transformation reactions. Other essential molecular descriptors are molar mass and molar volume, with properties such as critical temperature and pressure and molecular area being occasionally useful for specific purposes. A useful source of information and estimation methods on these properties is the handbook by Boethling and Mackay (2000).

Chemical identity may appear to present a trivial problem, but most chemicals have several names, and subtle differences between isomers (e.g., cis and trans) may be ignored. The most commonly accepted identifiers are the IUPAC name and the Chemical Abstracts System (CAS) number. More recently, methods have been sought of expressing the structure in line notation form so that computer entry of a series of symbols can be used to define a three-dimensional structure. For environmental purposes the SMILES (Simplified Molecular Identification and Line Entry System, Anderson et al. 1987) is favored, but the Wismesser Line Notation is also quite widely used.

Molar mass or molecular weight is readily obtained from structure. Also of interest for certain purposes are molecular volume and area, which may be estimated by a variety of methods.

When selecting physical-chemical properties or reactivity classes the authors have been guided by:

1. The acknowledgment of previous supporting or conflicting values,
2. The method of determination,
3. The perception of the objectives of the authors, not necessarily as an indication of competence, but often as an indication of the need of the authors to obtain accurate values, and
4. The reported values for structurally similar, or homologous compounds.

The literature contains a considerable volume of "calculated" data as distinct from experimental data. We have generally not included such data because they may be of questionable reliability. In some cases an exception has been made when no experimental data exist and the calculation is believed to provide a useful and reliable estimate.

### 1.2.2 Partitioning Properties

Solubility in water and vapor pressure are both "saturation" properties, i.e., they are measurements of the maximum capacity that a solvent phase has for dissolved chemical. Vapor pressure $\mathrm{P}(\mathrm{Pa})$ can be viewed as a "solubility in air," the corresponding concentration $\mathrm{C}\left(\mathrm{mol} / \mathrm{m}^{3}\right)$ being P/RT where R is the ideal gas constant ( $8.314 \mathrm{~J} / \mathrm{mol} . \mathrm{K}$ ) and T is absolute temperature $(\mathrm{K})$. Although most chemicals are present in the environment at concentrations well below saturation, these concentrations are useful for estimating air-water partition coefficients as ratios of saturation values. It is usually assumed
that the same partition coefficient applies at lower sub-saturation concentrations. Vapor pressure and solubility thus provide estimates of the air-water partition coefficient $\mathrm{K}_{\mathrm{Aw}}$, the dimensionless ratio of concentration in air (mass/volume) to that in water. The related Henry's law constant $\mathrm{H}\left(\mathrm{Pa} . \mathrm{m}^{3} / \mathrm{mol}\right)$ is the ratio of partial pressure in air $(\mathrm{Pa})$ to the concentration in water $\left(\mathrm{mol} / \mathrm{m}^{3}\right)$. Both express the relative air-water partitioning tendency.

When solubility and vapor pressure are both low in magnitude and thus difficult to measure, it is preferable to measure the air-water partition coefficient or Henry's law constant directly. It is noteworthy that atmospheric chemists frequently use $\mathrm{K}_{\mathrm{WA}}$, the ratio of water-to-air concentrations. This may also be referred to as the Henry's law constant.

The octanol-water partition coefficient $\mathrm{K}_{\mathrm{ow}}$ provides a direct estimate of hydrophobicity or of partitioning tendency from water to organic media such as lipids, waxes and natural organic matter such as humin or humic acid. It is invaluable as a method of estimating $\mathrm{K}_{\mathrm{OC}}$, the organic carbon-water partition coefficient, the usual correlation invoked being that of Karickhoff (1981)

$$
\mathrm{K}_{\mathrm{OC}}=0.41 \mathrm{~K}_{\mathrm{ow}}
$$

Seth et al. (1999) have suggested that a better correlation is

$$
\mathrm{K}_{\mathrm{OC}}=0.35 \mathrm{~K}_{\mathrm{ow}}
$$

and that the error limits on $\mathrm{K}_{\mathrm{OC}}$ resulting from differences in the nature of organic matter are a factor of 2.5 in both directions, i.e. the coefficient 0.35 may vary from 0.14 to 0.88 .
$\mathrm{K}_{\mathrm{OC}}$ is an important parameter which describes the potential for movement or mobility of pesticides in soil, sediment and groundwater. Because of the structural complexity of these agrochemical molecules, the above simple relationship which considers only the chemical's hydrophobicity may fail for polar and ionic compounds. The effects of pH , soil properties, mineral surfaces and other factors influencing sorption become important. Other quantities, $\mathrm{K}_{\mathrm{D}}$ (sorption partition coefficient to the whole soil on a dry weight basis) and $\mathrm{K}_{\mathrm{OM}}$ (organic matter-water partition coefficient) are also commonly used to describe the extent of sorption. $\mathrm{K}_{\mathrm{OM}}$ is often estimated as $0.56 \mathrm{~K}_{\mathrm{OC}}$, implying that organic matter is $56 \%$ carbon.
$\mathrm{K}_{\text {ow }}$ is also used to estimate equilibrium fish-water bioconcentration factors $\mathrm{K}_{\mathrm{B}}$, or BCF using a correlation similar to that of Mackay (1982)

$$
\mathrm{K}_{\mathrm{B}}=0.05 \mathrm{~K}_{\mathrm{ow}}
$$

where the term 0.05 corresponds to a lipid content of the fish of $5 \%$. The basis for this correlation is that lipids and octanol display very similar solvent properties, i.e., $\mathrm{K}_{\mathrm{LW}}$ (lipid-water) and $\mathrm{K}_{\mathrm{OW}}$ are equal. If the rate of metabolism is appreciable, equilibrium will not apply and the effective $\mathrm{K}_{\mathrm{B}}$ will be lower to an extent dictated by the relative rates of uptake and loss by metabolism and other clearance processes. If uptake is primarily from food, the corresponding bioaccumulation factor also depends on the concentration of the chemical in the food.

For dissociating chemicals it is essential to quantify the extent of dissociation as a function of pH using the dissociation constant $\mathrm{pK}_{\mathrm{a}}$. The parent and ionic forms behave and partition quite differently; thus pH and the presence of other ions may profoundly affect chemical fate. This is discussed later in more detail in Section 1.2.4.

The octanol-air partition coefficient $\mathrm{K}_{\mathrm{OA}}$ was originally introduced by Paterson et al. (1991) for describing the partitioning of chemicals from the atmosphere to foliage. It has proved invaluable for this purpose and for describing partitioning to aerosol particles and to soils. It can be determined experimentally using the technique devised by Harner and Mackay (1995). Although there are fewer data for $\mathrm{K}_{\mathrm{OA}}$ than for $\mathrm{K}_{\mathrm{OW}}$, its use is increasing and when available, data are included in this handbook. $\mathrm{K}_{\mathrm{OA}}$ has been applied to several situations involving partitioning of organic substances from the atmosphere to solid or liquid phases. Finizio et al. (1997) have shown that $\mathrm{K}_{\mathrm{OA}}$ is an excellent descriptor of partitioning to aerosol particles, while McLachlan et al. (1995) and Tolls and McLachlan (1994) have used it to describe partitioning to foliage, especially grasses. Hippelein and McLachlan (1998) have used $\mathrm{K}_{\mathrm{OA}}$ to describe partitioning between air and soil.

An attractive feature of $\mathrm{K}_{\mathrm{OA}}$ is that it can replace the liquid or supercooled liquid vapor pressure in a correlation. $\mathrm{K}_{\mathrm{OA}}$ is an experimentally measurable or accessible quantity, whereas the supercooled liquid vapor pressure must be estimated from the solid vapor pressure, the melting point and the entropy of fusion. The use of $\mathrm{K}_{\mathrm{OA}}$ thus avoids the potentially erroneous estimation of the fugacity ratio, i.e., the ratio of solid and liquid vapor pressures. This is especially important for solutes with high melting points and, thus, low fugacity ratios.

The availability of data on $\mathrm{K}_{\mathrm{AW}}, \mathrm{K}_{\mathrm{OW}}$ and $\mathrm{K}_{\mathrm{OA}}$ raises the possibility of a consistency test. At first sight it appears that $\mathrm{K}_{\mathrm{OA}}$ should equal $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, and indeed this is often approximately correct. The difficulty is that in the case of $\mathrm{K}_{\mathrm{AW}}$, the water phase is pure water, and for $\mathrm{K}_{\mathrm{OA}}$ the octanol phase is pure "dry" octanol. For $\mathrm{K}_{\mathrm{Ow}}$, the water phase inevitably contains dissolved octanol, and the octanol phase contains dissolved water and is thus not "dry." Beyer et al. (2002) and Cole and Mackay (2000) have discussed this issue.

If the partition coefficients are regarded as ratios of solubilities $S\left(\mathrm{~mol} / \mathrm{m}^{3}\right)$

$$
\begin{aligned}
& \mathrm{K}_{\mathrm{AW}}=\mathrm{S}_{\mathrm{A}} / \mathrm{S}_{\mathrm{W}} \text { or } \log \mathrm{K}_{\mathrm{AW}}=\log \mathrm{S}_{\mathrm{A}}-\log \mathrm{S}_{\mathrm{W}} \\
& \mathrm{~K}_{\mathrm{OA}}=\mathrm{S}_{\mathrm{O}} / \mathrm{S}_{\mathrm{A}} \text { or } \log \mathrm{K}_{\mathrm{OA}}=\log \mathrm{S}_{\mathrm{O}}-\log \mathrm{S}_{\mathrm{A}} \\
& \mathrm{~K}_{\mathrm{OW}}=\mathrm{S}_{\mathrm{OW}} / \mathrm{S}_{\mathrm{WO}} \text { or } \log \mathrm{K}_{\mathrm{OW}}=\log \mathrm{S}_{\mathrm{OW}}-\log \mathrm{S}_{\mathrm{WO}}
\end{aligned}
$$

where subscript A applies to the gas phase or air, W to pure water, O to dry octanol, OW to "wet" octanol and WO to water saturated with octanol. It follows that the assumption that $\mathrm{K}_{\mathrm{OA}}$ is $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$ is essentially that

$$
\begin{gathered}
\left(\log \mathrm{S}_{\mathrm{OW}}-\log \mathrm{S}_{\mathrm{O}}\right)-\left(\log \mathrm{S}_{\mathrm{WO}}-\log \mathrm{S}_{\mathrm{W}}\right)=0 \\
\text { or } \mathrm{S}_{\mathrm{OW}} \mathrm{~S}_{\mathrm{W}} /\left(\mathrm{S}_{\mathrm{O}} \cdot \mathrm{~S}_{\mathrm{WO}}\right) \text { is } 1.0
\end{gathered}
$$

This is obviously satisfied when $S_{\text {OW }}$ equals $S_{O}$ and $S_{\text {wo }}$ equals $S_{W}$, but this is not necessarily valid, especially when $K_{\text {ow }}$ is large.

There are apparently two sources of this effect. The molar volume of water changes relatively little as a result of the presence of a small quantity of dissolved octanol, however the quantity of dissolved water in the octanol is considerable, causing a reduction in molar volume of the octanol phase. The result is that even if activity coefficients are unaffected, $\log \mathrm{S}_{\mathrm{O}} / \mathrm{S}_{\mathrm{w}}$ will be about 0.1 units less than that of $\log \mathrm{K}_{\mathrm{ow}}$. Effectively, the octanol phase "swells" as a result of the presence of water, and the concentration is reduced. In addition, when $\log \mathrm{K}_{\mathrm{ow}}$ exceeds 4.0 there is an apparent effect on the activity coefficients which causes $\log \left(\mathrm{S}_{\mathrm{O}} / \mathrm{S}_{\mathrm{w}}\right)$ to increase. This increase can amount to about one $\log$ unit when log $\mathrm{K}_{\mathrm{OW}}$ is about 8. A relatively simple correlation based on the analysis by Beyer et al. (2002) (but differing from their correlation) is that

$$
\log \mathrm{K}_{\mathrm{OA}}=\log \left(\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}\right)-0.10+\left[0.30 \log \mathrm{~K}_{\mathrm{OW}}-1.20\right]
$$

when $\log \mathrm{K}_{\mathrm{Ow}}$ is 4 or less the term in square brackets is ignored
when $\log \mathrm{K}_{\mathrm{ow}}$ is 4 or greater that term is included

### 1.2.3 Temperature Dependence

All partitioning properties change with temperature. The partition coefficients, vapor pressure, $\mathrm{K}_{\mathrm{AW}}$ and $\mathrm{K}_{\mathrm{OA}}$, are more sensitive to temperature variation because of the large enthalpy change associated with transfer to the vapor phase. The simplest general expression theoretically based temperature dependence correlation is derived from the integrated Clausius-Clapeyron equation, or van't Hoff form expressing the effect of temperature on an equilibrium constant $K_{p}$,

$$
R \cdot \ln K_{p}=A_{o}-B / T
$$

which can be rewritten as

$$
\ln (\text { Property })=A-\Delta H / R T
$$

where $A_{o}, B$ and $A$ are constants, $\Delta H$ is the enthalpy of the phase change, i.e., evaporation from pure state for vapor pressure, dissolution from pure state into water for solubility, and for air-water transition in the case of Henry's law constant.

The fit is improved by adding further coefficients in additional terms. The variation of these equilibrium constants with temperature can be expressed by (Clarke and Glew 1966),

$$
R \cdot \ln K_{p}(T)=A+B / T+C \cdot \ln T+D T+E T^{2}+F T^{3}+\ldots \ldots
$$

where $A, B, C, D, E, F$ are constants.
There have been numerous approaches to describing the temperature dependence of the properties. For aqueous solubility, the most common expression is the van't Hoff equation of the form (Hildebrand et al. 1970):

$$
d(\ln x) / d(1 / T)=-\Delta_{\mathrm{sol}} H / R
$$

where $x$ is the mole fraction solubility, $T$ is the temperature in $\mathrm{K}, R$ is the ideal gas constant, and $\Delta_{\text {sol }} H$ is the enthalpy of solution of the solute. The enthalpy of solution can be considered as the sum of various contributions such as cavity formation and interactions between solute-solute or solute-solvent as discussed by Bohon and Claussen (1951), Arnold et al. (1958), Owen et al. (1986) and many others. Assuming the enthalpy of solution is constant over a narrow temperature range, integrating gives,

$$
\ln x=-\Delta_{\text {sol }} H / R T+C
$$

where $C$ is a constant.
The relation between aqueous solubility and temperature is complicated because of the nature of the interactions between the solute and water structure. The enthalpy of solution can vary greatly with temperature, e.g., some liquid aromatic hydrocarbons display a minimum solubility corresponding to zero enthalpy of solution between 285 and 320 K. For instance, benzene has a minimum solubility at 291 K (Bohon and Claussen 1951, Arnold et al. 1958, Shaw 1989a) and alkylbenzenes display similar behavior (Shaw 1989a,b, Owens 1986). As is illustrated later in chapter 3, solid aromatic hydrocarbons show a slight curvature in plots of logarithm of mole fraction solubility versus reciprocal absolute temperature. For narrow ranges in environmental temperatures, the enthalpy of solution may be assumed to be constant, and the linear van't Hoff plot of $\ln x$ versus $1 / T$ is often used (Dickhut et al. 1986). Other relationships such as quadratic or cubic equations have been reported (May et al. 1978), and polynomial series (Clarke and Glew 1966, May et al. 1983, Owens et al. 1986) have been used when the data justify such treatment.

Equations relating vapor pressure to temperature are usually based on the two-parameter Clausius-Clapeyron equation,

$$
d\left(\ln P^{S}\right) / d T=\Delta_{\mathrm{vap}} H / R T^{2}
$$

where $P^{S}$ is vapor pressure, $\Delta_{\text {vap }} H$ is the enthalpy of vaporization. Again assuming $\Delta_{\text {vap }} H$ is constant over a narrow range of temperature, this gives,

$$
\ln P^{S}=-\Delta_{\mathrm{vap}} H / R T+C
$$

which can be rewritten as the Clapeyron equation

$$
\log P^{S}=A-B / T
$$

This can be empirically modified by introducing additional parameters to give the three-parameter Antoine equation by replacing $T$ with $(T+C)$, where $C$ is a constant, which is the most common vapor pressure correlation used to represent experimental data (Zwolinski and Wilhoit 1971, Boublik et al. 1984, Stephenson and Malanowski 1987, and other handbooks).

$$
\log P^{S}=A-B /(t+C)
$$

where $A, B$ and $C$ are constants and $t$ often has units of ${ }^{\circ} \mathrm{C}$.
Other forms of vapor pressure equations, such as Cox equation (Osborn and Douslin 1974, Chao et al. 1983), Chebyshev polynomial (Ambrose 1981), Wagner's equation (Ambrose 1986), have also been widely used. Although
the enthalpy of vaporization varies with temperature, for the narrow environmental temperature range considered in environmental conditions, it is often assumed to be constant, for example, for the more volatile monoaromatic hydrocarbons and the less volatile polynuclear aromatic hydrocarbons.

The van't Hoff equation also has been used to describe the temperature effect on Henry's law constant over a narrow range for volatile chlorinated organic chemicals (Ashworth et al. 1988) and chlorobenzenes, polychlorinated biphenyls, and polynuclear aromatic hydrocarbons (ten Hulscher et al. 1992, Alaee et al. 1996). Henry's law constant can be expressed as the ratio of vapor pressure to solubility, i.e., $p / c$ or $p / x$ for dilute solutions. Note that since H is expressed using a volumetric concentration, it is also affected by the effect of temperature on liquid density whereas $k_{H}$ using mole fraction is unaffected by liquid density (Tucker and Christian 1979), thus

$$
\begin{gathered}
\ln \left(k_{H} / P a\right)=\ln \left[\left(P^{S} / P a\right) / x\right] \\
\ln \left(H / \mathrm{Pa} \cdot \mathrm{~m}^{3} \cdot \mathrm{~mol}^{-1}\right)=\ln \left[\left(P^{S} / P a\right) /\left(C_{W}^{S} / \mathrm{mol} \cdot \mathrm{~m}^{-3}\right)\right]
\end{gathered}
$$

where $C^{S}{ }_{W}$ is the aqueous solubility.
By substituting equations for vapor pressure and solubility, the temperature dependence equation for Henry's law constant can be obtained, as demonstrated by Glew and Robertson (1956), Tsonopoulos and Wilson (1983), Heiman et al. (1985), and ten Hulscher et al. (1991).

Care must be taken to ensure that the correlation equations are applied correctly, especially since the units of the property, the units of temperature and whether the logarithm is base e or base 10 . The equations should not be used to extrapolate beyond the stated temperature range.

### 1.2.4 Treatment of Dissociating Compounds

In the case of dissociating or ionizing organic chemicals such as organic acids and bases, e.g., phenols, carboxylic acids and amines, it is desirable to calculate the concentrations of ionic and non-ionic species, and correct for this effect. A number of authors have discussed and reviewed the effect of pH and ionic strength on the distribution of these chemicals in the environment, including Westall et al. (1985), Schwarzenbach et al. (1988), Jafvert et al. (1990), Johnson and Westall (1990) and the text by Schwarzenbach, Gschwend and Imboden (1993).

A simple approach is suggested here for estimating the effect of pH on properties and environmental fate using the phenols as an example. A similar approach can be used for bases. The extent of dissociation is characterized by the acid dissociation constant, $K_{\mathrm{a}}$, expressed as its negative logarithm, $\mathrm{pK}_{\mathrm{a}}$, which for most chloro-phenolic compounds range between 4.75 for pentachlorophenol and 10.2 to phenol, and between 10.0 and 10.6 for the alkylphenols. The dissolved concentration in water is thus the sum of the undissociated, parent or protonated compound and the dissociated phenolate ionic form. When the $\mathrm{pK}_{\mathrm{a}}$ exceeds pH by 2 or more units, dissociation is $1 \%$ or less and for most purposes is negligible. The ratio of ionic to non-ionic or dissociated to undissociated species concentrations is given by,

$$
\text { ionic/non-ionic }=10^{(\mathrm{pH}-\mathrm{pKa})}=I
$$

The fraction ionic $x_{\mathrm{I}}$ is $I /(1+I)$. The fraction non-ionic $x_{\mathrm{N}}$ is $1 /(1+I)$. For compounds such as pentachlorophenol in which pH generally exceeds $\mathrm{pK}_{\mathrm{a}}, I$ and $x_{\mathrm{I}}$ can be appreciable, and there is an apparently enhanced solubility (Horvath and Getzen 1985, NRCC 1982, Yoshida et al. 1987, Arcand et al. 1995, Huang et al. 2000). There are other reports of pH effects on octanol-water partition coefficient (Kaiser and Valdmanis 1982, Westall et al. 1985, Lee et al. 1990, Smejtek and Wang 1993), soil sorption behavior (Choi and Amoine 1974, Lee et al. 1990, Schellenberg et al. 1984, Yoshida et al. 1987, Lee et al. 1990), bioconcentration and uptake kinetics to goldfish (Stehly and Hayton 1990) and toxicity to algae (Smith et al. 1987, Shigeoka et al. 1988).

The following treatment has been suggested by Shiu et al. (1994) and is reproduced briefly below. The simplest, "first-order" approach is to take into account the effect of dissociation by deducing the ratio of ionic to non-ionic species $I$, the fraction ionic $x_{\mathrm{I}}$ and the fraction non-ionic $x_{\mathrm{N}}$ for the chemical at both the pH and temperature of experimental data determination ( $I_{\mathrm{D}}, x_{\mathrm{ID}}, x_{\mathrm{ND}}$ ) and at the pH and temperature of the desired environmental simulation ( $I_{\mathrm{E}}, x_{\mathrm{IE}}, x_{\mathrm{NE}}$ ). It is assumed that dissociation takes place only in aqueous solution, not in air, organic carbon, octanol or lipid phases. Some ions and ion pairs are known to exist in the latter two phases, but there are insufficient data to justify a general procedure for estimating the quantities. No correction is made for the effect of cations other than $\mathrm{H}^{+}$. This approach must be regarded as merely a first correction for the dissociation effect. An accurate evaluation should preferably be based on experimental
determinations. The reported solubility $C \mathrm{~mol} / \mathrm{m}^{3}$ and $\mathrm{K}_{\mathrm{ow}}$ presumably refer to the total of ionic and non-ionic forms, i.e., $C_{\mathrm{T}}$ and $\mathrm{K}_{\mathrm{ow}, \mathrm{T}}$, at the pH of experimental determination, i.e.,

$$
C_{\mathrm{T}}=C_{\mathrm{N}}+C_{\mathrm{I}}
$$

The solubility and $K_{\text {ow }}$ of the non-ionic forms can be estimated as

$$
C_{\mathrm{N}}=C_{\mathrm{T}} \cdot x_{\mathrm{ND}} ; \quad K_{\mathrm{OW}, \mathrm{~N}}=K_{\mathrm{OW}, \mathrm{~T}} / x_{\mathrm{ND}}
$$

Vapor pressure $P^{\mathrm{s}}$ is not affected, but the apparent Henry's law constant $H_{\mathrm{T}}$, must also be adjusted to $H_{\mathrm{T}} / x_{\mathrm{N}}$, being $P^{\mathrm{S}} / C_{\mathrm{N}}$ or $P^{s} /\left(C_{\mathrm{T}} \cdot x_{\mathrm{N}}\right)$.
$C_{N}$ and $K_{\text {OWWN }}$ can be applied to environmental conditions with a temperature adjustment if necessary. Values of $I_{E} x_{I x}$ and $x_{N E}$ can be deduced from the environmental pH and the solubility and $K_{O W}$ of the total ionic and non-ionic forms calculated.

In the tabulated data presented in this handbook the aqueous solubilities selected are generally those estimated to be of the non-ionic form unless otherwise stated.

### 1.2.5 Treatment of Water-Miscible Compounds

In the multimedia models used in this series of volumes, an air-water partition coefficient $K_{\mathrm{AW}}$ or Henry's law constant $(H)$ is required and is calculated from the ratio of the pure substance vapor pressure and aqueous solubility. This method is widely used for hydrophobic chemicals but is inappropriate for water-miscible chemicals for which no solubility can be measured. Examples are the lower alcohols, acids, amines and ketones. There are reported "calculated" or "pseudo-solubilities" that have been derived from QSPR correlations with molecular descriptors for alcohols, aldehydes and amines (by Leahy 1986; Kamlet et al. 1987, 1988 and Nirmalakhandan and Speece 1988a,b). The obvious option is to input the $H$ or $K_{A W}$ directly. If the chemical's activity coefficient $\gamma$ in water is known, then $H$ can be estimated as $v_{\mathrm{w}} \gamma P_{\mathrm{L}}^{\mathrm{S}}$, where $v_{\mathrm{w}}$ is the molar volume of water and $P_{\mathrm{L}}^{\mathrm{S}}$ is the liquid vapor pressure. Since $H$ can be regarded as $P_{\mathrm{L}}^{\mathrm{S}} / C_{\mathrm{L}}^{\mathrm{S}}$, where $C_{\mathrm{L}}^{\mathrm{S}}$ is the solubility, it is apparent that ( $1 / v_{\mathrm{w}} \gamma$ ) is a " pseudo -solubility." Correlations and measurements of $\gamma$ are available in the physical-chemical literature. For example, if $\gamma$ is 5.0 , the pseudo-solubility is $11100 \mathrm{~mol} / \mathrm{m}^{3}$ since the molar volume of water $v_{\mathrm{w}}$ is $18 \times 10^{-6} \mathrm{~m}^{3} / \mathrm{mol}$ or $18 \mathrm{~cm}^{3} / \mathrm{mol}$. Chemicals with $\gamma$ less than about 20 are usually miscible in water. If the liquid vapor pressure in this case is $1000 \mathrm{~Pa}, H$ will be $1000 / 11100$ or $0.090 \mathrm{~Pa} \cdot \mathrm{~m}^{3} / \mathrm{mol}$ and $K_{\mathrm{AW}}$ will be $H / R T$ or $3.6 \times 10^{-5}$ at $25^{\circ} \mathrm{C}$. Alternatively, if $H$ or $K_{\mathrm{AW}}$ is known, $C_{\mathrm{L}}^{\mathrm{S}}$ can be calculated. It is possible to apply existing models to hydrophilic chemicals if this pseudo-solubility is calculated from the activity coefficient or from a known $H$ (i.e., $C_{\mathrm{L}}^{\mathrm{S}}, P_{\mathrm{L}}^{\mathrm{S}} / H$ or $P_{\mathrm{L}}^{\mathrm{S}}$ or $K_{\mathrm{AW}} \cdot R T$ ). This approach is used here. In the fugacity model illustrations all pseudo-solubilities are so designated and should not be regarded as real, experimentally accessible quantities.

### 1.2.6 Treatment of Partially Miscible Substances

Most hydrophobic substances have low solubilities in water, and in the case of liquids, water is also sparingly soluble in the pure substance. Some substances such as butanols and chlorophenols display relatively high mutual solubilities. As temperature increases, these mutual solubilities increase until a point of total miscibility is reached at a critical solution temperature. Above this temperature, no mutual solubilities exist. A simple plot of solubility versus temperature thus ends at this critical point. At low temperatures near freezing, the phase diagram also become complex. Example of such systems have been reported for sec-butyl alcohol (2-butanol) by Ochi et al. (1996) and for chlorophenols by Jaoui et al. (1999).

### 1.2.7 Treatment of Gases and Vapors

A volatile substance may exist in one of three broad classes that can be loosely termed gases, vapors and liquids.
A gaseous substance such as oxygen at normal environmental conditions exists at a temperature exceeding its critical temperature of 155 K . No vapor pressure can be defined or measured under this super-critical condition, thus no Henry's law constant can be calculated. Empirical data are required.

A substance such as propane with a critical temperature of 370 K has a measurable vapor pressure of 998000 Pa , or approximately 10 atm at $27^{\circ} \mathrm{C}$, which exceeds atmospheric pressure of 101325 Pa , the boiling point being $-42^{\circ} \mathrm{C}$ or 231 K . It is thus a vapor at normal temperatures and pressures. A Henry's law constant can be calculated from this vapor pressure and a solubility as described earlier.

Most substances treated in this handbook are liquids or solids at environmental conditions; thus their boiling points exceed $25^{\circ} \mathrm{C}$. Benzene, for example, has a critical temperature of 562 K , a boiling point of $80^{\circ} \mathrm{C}$ and a vapor pressure of 12700 Pa at $25^{\circ} \mathrm{C}$.

When a solubility in water is measured and reported for gases and vapors an ambiguity is possible. For gases the solubility and the corresponding partial or total pressure in the gas phase must be reported since the solubility is dependent on this pressure as dictated by Henry's Law. For liquids and solids the solubility is presumably measured under conditions when the partial pressure equals the vapor pressure. For vapors such as propane the solubility can be measured either at a specified pressure (usually 1 atmosphere) or under high-pressure conditions (e.g., 10 atm ) when the substance is a liquid. When calculating $H$ or $K_{A W}$ it is essential to use the correct pressure corresponding to the solubility measurement. Care must be exercised when treating substances with boiling points at or below environmental temperatures to ensure that the solubility is interpreted and used correctly.

### 1.2.8 Solids, Liquids and the Fugacity Ratio

Saturation properties such as solubility in water and vapor pressure can be measured directly for solids and liquids. For certain purposes it is useful to estimate the solubility that a solid substance would have if it were liquid at a temperature below the melting point. For example, naphthalene melts at $80^{\circ} \mathrm{C}$ and at $25^{\circ} \mathrm{C}$ the solid has a solubility in water of $33 \mathrm{~g} / \mathrm{m}^{3}$ and a vapor pressure of 10.9 Pa . If naphthalene was a liquid at $25^{\circ} \mathrm{C}$ it is estimated that its solubility would be $115 \mathrm{~g} / \mathrm{m}^{3}$ and its vapor pressure 38.1 Pa , both a factor of 3.5 greater. This ratio of solid to liquid solubilities or vapor pressures is referred to as the fugacity ratio. It is 1.0 at the melting point and falls, in this case at lower temperatures to 0.286 at $25^{\circ} \mathrm{C}$.

Solubilities and vapor pressures of a solid substance in the liquid state are often reported for the following four reasons.

Measurements of gas chromatographic retention time are often used as a fast and easy method of estimating vapor pressure. These estimated pressures are related to the gas/substrate partition coefficient, which can be regarded as a ratio of solubility of the substance in the gas to that in the substrate, both solubilities being of the substance in the liquid state. As a result the estimated vapor pressures are of the liquid state. To obtain the solid vapor pressure requires multiplication by the fugacity ratio. It is important to establish if the estimated and reported property is of the vapor or liquid.

QSPRs in which solubilities and vapor pressures are correlated against molecular structure are done exclusively using the liquid state property. This avoids the complication introduced by the effect of fugacity ratio or melting point on the solid state property.

When a solid is in liquid solution it behaves according to its liquid state properties because it is in a liquid mixture. When applying Raoult's Law or similar expressions, the pure substance property is that of the liquid. Liquids such as crude oils and PCB mixtures consist largely of solid substances, but they are in the liquid state and generally unable to precipitate as solid crystals because of their low individual concentrations.

When estimating air-aerosol partitioning of gas phase substances such as PAHs, most of which are solids, it is usual to use the liquid state vapor pressure as the correlating parameter. This is because the PAH is effectively in a liquidlike state on or in the aerosol particle. It does not exist in crystalline form.

When calculating partition coefficients such as $\mathrm{K}_{\mathrm{AW}}, \mathrm{K}_{\mathrm{OW}}$ or $\mathrm{K}_{\mathrm{OA}}$ from solubilities it is immaterial if the values used are of solids or liquids, but it is erroneous to mix the two states, e.g., a solid solubility and a liquid vapor pressure.

The fugacity ratio F can be estimated at temperature $\mathrm{T}(\mathrm{K})$ from the expression

$$
\ln \mathrm{F}=-\Delta \mathrm{S}\left(\mathrm{~T}_{\mathrm{M}}-\mathrm{T}\right) / \mathrm{RT}
$$

where $\Delta \mathrm{S}$ is the entropy of fusion, $\mathrm{T}_{\mathrm{M}}$ is the melting point, and R is the gas constant. $\Delta \mathrm{S}$ is related to the measurable enthalpy of fusion $\Delta \mathrm{H}$ at the melting point as $\Delta \mathrm{H} / \mathrm{T}_{\mathrm{M}}$. The reader should use experimental data for $\Delta \mathrm{H}, \Delta \mathrm{S}$ and melting point whenever possible. The most reliable method is to measure $\Delta \mathrm{H}$ calorimetrically, calculate $\Delta \mathrm{S}$ and use this value to estimate F . Only in the absence of $\Delta \mathrm{H}$ data should a QSPR be used or Walden's Rule applied that $\Delta \mathrm{S}$ is approximately $56.5 \mathrm{~J} / \mathrm{mol} \mathrm{K}$. This assumption leads to the equations

$$
\mathrm{F}=\exp \left(-6.79\left(\mathrm{~T}_{\mathrm{M}} / \mathrm{T}-1\right)\right)
$$

$\log \mathrm{F}=-0.01\left(\mathrm{~T}_{\mathrm{M}}-298\right)$

F is thus 1.0 at the melting point, with lower values at lower temperatures. It is not applied at temperatures exceeding $\mathrm{T}_{\mathrm{M}}$. This issue is discussed by Mackay (2001), Tesconi and Yalkowsky (2000), Yalkowsky and Banerjee (1992) and Chickos et al. (1999).

### 1.2.9 Chemical Reactivity and Half-Lives

Characterization of chemical reactivity presents a challenging problem in environmental science in general and especially in handbooks. Whereas radioisotopes have fixed half-lives, the half-life of a chemical in the environment depends not only on the intrinsic properties of the chemical, but also on the nature of the environmental compartments. Factors such as sunlight intensity, hydroxyl radical concentration and the nature of the microbial community, as well as temperature, affect the chemical's half-life so it is impossible (and misleading) to document a single reliable half-life. We suggest that the best approach is to suggest a semi-quantitative classification of half-lives into groups or ranges, assuming average environmental conditions to apply. Obviously, a different class will generally apply between compartments such as in air and bottom sediment. In this compilation we use the following class ranges for chemical reactivity in a single medium such as water.

These times are divided logarithmically with a factor of approximately 3 between adjacent classes. With the present state of knowledge it is probably misleading to divide the classes into finer groupings; indeed, a single chemical is likely to experience half-lives ranging over three classes, depending on season. These half-lives apply to the reaction of the parent substance. Often a degradation product or metabolite is formed that is of environmental concern. Since it has different properties it requires separate assessment. The ultimate degradation to inorganic species may require a much longer time than is indicated by the initial half-life.

| class | mean half-life (hours) | range (hours) |
| :--- | :--- | :--- |
| 1 | $5<10$ |  |
| 2 | $17(\sim 1$ day $)$ | $10-30$ |
| 3 | $55(\sim 2$ days $)$ | $30-100$ |
| 4 | $170(\sim 1$ week $)$ | $100-300$ |
| 5 | $550(\sim 3$ weeks $)$ | $300-1,000$ |
| 6 | $1700(\sim 2$ months $)$ | $1,000-3,000$ |
| 7 | $5500(\sim 8$ months $)$ | $3,000-10,000$ |
| 8 | $17000(\sim 2$ years $)$ | $10,000-30,000$ |
| 9 | $55000(\sim 6$ years $)$ | $30,000-100,000$ |
| 10 | $>11$ years | $>100,000$ |

When compiling the suggested reactivity classes, the authors have examined the available information on reaction rates of the chemical in each medium by all relevant processes. These were expressed as an overall half-life for transformation. The product of the half-life and the corresponding rate constant is $\ln 2$ or 0.693 . For example, a chemical may be subject to biodegradation with a half-life of 20 days or 480 hours (rate constant $0.0014 \mathrm{~h}^{-1}$ ) and simultaneous photolysis with a rate constant of $0.0011 \mathrm{~h}^{-1}$ (half-life 630 hours). The overall rate constant is thus $0.0025 \mathrm{~h}^{-1}$ and the half-life is 277 hours or 12 days. Data for homologous chemicals have also been compiled, and insights into the reactivity of various functional groups considered. In most cases a single reaction class is assigned to the series; in the above case, class 4 with a mean half-life of 170 hours would be chosen. These half-lives must be used with caution, and it is wise to test the implications of selecting longer and shorter half-lives.

The most reliable kinetic data are for atmospheric oxidation by hydroxyl radicals. These data are usually reported as second-order rate constants applied to the concentration of the chemical and the concentration of hydroxyl radicals (usually of the order of $10^{6}$ radicals per $\mathrm{cm}^{3}$ ). The product of the assumed hydroxyl radical concentration and the secondorder rate constant is a first-order rate constant from which a half-life can be deduced.

Extensive research has been conducted into the atmospheric chemistry of organic chemicals because of air quality concerns. Recently, Atkinson and coworkers (1984, 1985, 1987, 1988, 1989, 1990, 1991), Altshuller (1980, 1991) and Sabljic and Güsten (1990) have reviewed the photochemistry of many organic chemicals of environmental interest for their gas phase reactions with hydroxyl radicals $(\mathrm{OH})$, ozone $\left(\mathrm{O}_{3}\right)$ and nitrate radicals $\left(\mathrm{NO}_{3}\right)$ and have provided detailed information on reaction rate constants and experimental conditions, which allowed the estimation of atmospheric lifetimes. Klöpffer (1991) has estimated the atmospheric lifetimes for the reaction with OH radicals to range from 1 hour to 130 years, based on these reaction rate constants and an assumed constant concentration of OH
radicals in air. As Atkinson (1985) has pointed out, the gas phase reactions with OH radicals are the major tropospheric loss process for the alkanes, haloalkanes, the lower alkenes, the aromatic hydrocarbons, and a majority of the oxygencontaining organics. In addition, photooxidation reactions with $\mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ radicals can result in transformation of these compounds. The night-time reaction with $\mathrm{NO}_{3}$ radicals may also be important (Atkinson and Carter 1984, Sabljic and Güsten 1990).

There are fewer studies on direct or indirect photochemical degradation in the water phase; however, Klöpffer (1991) had pointed out that the rate constant or lifetimes derived from these studies "is valid only for the top layer or surface waters." Mill $(1982,1989,1993)$ and Mill and Mabey (1985) have estimated half-lives of various chemicals in aqueous solutions from their reaction rate constants with singlet oxygen, as well as photooxidation with hydroxyl and peroxy radicals. Buxton et al. (1988) gave a critical review of rate constants for reactions with hydrated electrons, hydrogen atoms and hydroxyl radicals in aqueous solutions. Mabey and Mill (1978) also reviewed the hydrolysis of organic chemicals in water under environmental conditions. Recently, Ellington and coworkers (1987a,b, 1988, 1989) also reported the hydrolysis rate constants in aqueous solutions for a variety of organic chemicals.

In most cases, a review of the literature suggested that reaction rates in water by chemical processes are 1 to 2 orders of magnitude slower than in air, but with biodegradation often being significant, especially for hydrocarbons and oxygen-containing chemicals. Generally, the water half-life class is three more than that in air, i.e., a factor of about 30 slower. Chemicals in soils tend to be shielded from photolytic processes, and they are less bioavailable, thus the authors have frequently assigned a reactivity class to soil of one more than that for water. Bottom sediments are assigned an additional class to that of soils largely on the basis that there is little or no photolysis, there may be lack of oxygen, and the intimate sorption to sediments renders the chemicals less bioavailable.

Because of the requirements of regulations for certain chemicals such as pesticides, extensive data usually exist on partitioning properties and reactivity or half-lives of active ingredients. In some cases these data have been peer-reviewed and published in the scientific literature, but often they are not generally available. A reader with interest in a specific pesticide can often obtain additional data from manufacturers or from registration literature, including accounts of chemical fate under field application conditions. Frequently these data are used as input to pesticide fate models, and the results of these modeling exercises may be available or published in the scientific literature.

The chemical reactivity of these substances is a topic which continues to be the subject of extensive research; thus there is often detailed, more recent information about the fate of chemical species which are of particular relevance to air or water quality. The reader is thus urged to consult the original and recent references because when considering the entire multimedia picture, it is impossible in a volume such as this to treat this subject in the detail it deserves.

### 1.3 EXPERIMENTAL METHODS

### 1.3.1 Solubility in Water and pK ${ }_{\mathrm{a}}$

Most conventional organic contaminants are fairly hydrophobic and thus exhibit a low but measurable solubility in water. Solubility is often used to estimate the air-water partition coefficient or Henry's law constant, but this is not possible for miscible chemicals; indeed the method is suspect for chemicals of appreciable solubility in water, i.e., exceeding $1 \mathrm{~g} / 100 \mathrm{~g}$. Direct measurement of the Henry's law constant is thus required.

The conventional method of preparing saturated solutions for the determination of solubility is batch equilibration. An excess amount of solute chemical is added to water and equilibrium is achieved by shaking gently (generally referred as the "shake flask method") or slow stirring with a magnetic stirrer. The aim is to prevent formation of emulsions or suspensions and thus avoid extra experimental procedures such as filtration or centrifuging which may be required to ensure that a true solution is obtained. Experimental difficulties can still occur with sparingly soluble chemicals such as longer chain alkanes and polycyclic aromatic hydrocarbons (PAHs) because of the formation of emulsion or microcrystal suspensions. An alternative approach is to coat a thin layer of the chemical on the surface of the equilibration flask before water is added. An accurate "generator column" method is also used (Weil et al. 1974, May et al. 1978a,b) in which a column is packed with an inert solid support, such as glass beads and then coated with the solute chemical. Water is pumped through the column at a controlled, known flow rate to achieve saturation.

The method of concentration measurement of the saturated solution depends on the solute solubility and its chemical properties. Some common methods used for solubility measurement are listed below.

1. Gravimetric or volumetric methods (Booth and Everson 1948)

An excess amount of solid compound is added to a flask containing water to achieve saturation solution by shaking, stirring, centrifuging until the water is saturated with solute and undissolved solid or liquid
residue appears, often as a cloudy phase. For liquids, successive known amounts of solute may be added to water and allowed to reach equilibrium, and the volume of excess undissolved solute is measured.
2. Instrumental methods
a. UV spectrometry (Andrews and Keefer 1950, Bohon and Claussen 1951, Yalkowsky and Valvani 1976);
b. Gas chromatographic analysis with FID, ECD or other detectors (McAuliffe 1966, Mackay et al. 1975, Chiou et al. 1982, Bowman and Sans 1983);
c. Fluorescence spectrophotometry (Mackay and Shiu 1977);
d. Interferometry (Gross and Saylor 1931);
e. High-pressure liquid chromatography (HPLC) with I.R., UV or fluorescence detection (May et al. 1978a,b, Wasik et al. 1983, Shiu et al. 1988, Doucette and Andren 1988a);
f. Liquid phase elution chromatography (Schwarz 1980, Schwarz and Miller 1980);
g. Nephelometric methods (Davis and Parke 1942, Davis et al. 1942, Hollifield 1979);
h. Radiotracer or liquid scintillation counting (LSC) method (Banerjee et al. 1980, Lo et al. 1986).

For most organic chemicals the solubility is reported at a defined temperature in distilled water. For substances which dissociate (e.g., phenols, carboxylic acids and amines) it is essential to report the pH of the determination because the extent of dissociation affects the solubility. It is common to maintain the desired pH by buffering with an appropriate electrolyte mixture. This raises the complication that the presence of electrolytes modifies the water structure and changes the solubility. The effect is usually "salting-out." For example, many hydrocarbons have solubilities in seawater about 75\% of their solubilities in distilled water. Care must thus be taken to interpret and use reported data properly when electrolytes are present.

The dissociation constant $\mathrm{K}_{\mathrm{a}}$ or its commonly reported negative logarithmic form $\mathrm{pK}_{\mathrm{a}}$ is determined in principle by simultaneous measurement or deduction of the ionic and non-ionic concentrations and the pH of the solution.

The most common problem encountered with reported data is inaccuracy associated with very low solubilities, i.e., those less than $1.0 \mathrm{mg} / \mathrm{L}$. Such solutions are difficult to prepare, handle and analyze, and reported data often contain appreciable errors.

As was discussed earlier, care must be taken when interpreting solubility data for gases, i.e., substances for which the temperature exceeds the boiling point. Solubility then depends on the pressure which may be atmospheric or the higher vapor pressure.

### 1.3.2 Vapor Pressure

In principle, the determination of vapor pressure involves the measurement of the saturation concentration or pressure of the solute in a gas phase. The most reliable methods involve direct determination of these concentrations, but convenient indirect methods are also available based on evaporation rate measurements or chromatographic retention times. Some methods and approaches are listed below.
a. Static method, the equilibrium pressure in a thermostatic vessel is directly measured by use of pressure gauges: diaphragm gauge (Ambrose et al. 1975), Rodebush gauge (Sears and Hopke 1947), inclined-piston gauge (Osborn and Douslin 1975);
b. Dynamic method (or boiling point) for measuring relatively high vapor pressure, eg., comparative ebulliometry (Ambrose 1981);
c. Effusion methods, torsion and weight-loss (Balson 1947, Bradley and Cleasby 1953, Hamaker and Kerlinger 1969, De Kruif 1980);
d. Gas saturation or transpiration methods (Spencer and Cliath 1970, 1972, Sinke 1974, Macknick and Prausnitz 1979, Westcott et al. 1981, Rordorf 1985a,b, 1986);
e. Dynamic coupled-column liquid chromatographic method- a gas saturation method (Sonnefeld et al. 1983);
f. Calculation from evaporation rates and vapor pressures of a reference compound (Gückel et al. 1974, 1982, Dobbs and Grant 1980, Dobbs and Cull 1982);
g. Calculation from GC retention time data (Hamilton 1980, Westcott and Bidleman 1982, Bidleman 1984, Kim et al. 1984, Foreman and Bidleman 1985, Burkhard et al. 1985a, Hinckley et al. 1990).

The greatest difficulty and uncertainty arises when determining the vapor pressure of chemicals of low volatility, i.e., those with vapor pressures below 1.0 Pa. Vapor pressures are strongly dependent on temperature, thus accurate temperature control is essential. Data are often regressed against temperature and reported as Antoine or Clapeyron constants. Care
must be taken if the Antoine or other equations are used to extrapolate data beyond the temperature range specified. It must be clear if the data apply to the solid or liquid phase of the chemical.

### 1.3.3 Octanol-Water Partition Coefficient K

The experimental approaches are similar to those for solubility, i.e., employing shake flask or generator-column techniques. Concentrations in both the water and octanol phases may be determined after equilibration. Both phases can then be analyzed by the instrumental methods discussed above and the partition coefficient is calculated from the concentration ratio $C_{\mathrm{O}} / C_{\mathrm{w}}$. This is actually the ratio of solute concentration in octanol saturated with water to that in water saturated with octanol.

As with solubility, $K_{\mathrm{OW}}$ is a function of the presence of electrolytes and for dissociating chemicals it is a function of pH . Accurate values can generally be measured up to about $10^{7}$, but accurate measurement beyond this requires meticulous technique. A common problem is the presence of small quantities of emulsified octanol in the water phase. The high concentration of chemical in that emulsion causes an erroneously high apparent water phase concentration.

Considerable success has been achieved by calculating $K_{\mathrm{OW}}$ from molecular structure; thus, there has been a tendency to calculate $K_{\text {OW }}$ rather than measure it, especially for "difficult" hydrophobic chemicals. These calculations are, in some cases, extrapolations and can be in serious error. Any calculated $\log \mathrm{K}_{\mathrm{ow}}$ value above 7 should be regarded as suspect, and any experimental or calculated value above 8 should be treated with extreme caution.

For many hydrophilic compounds such as the alcohols, $\mathrm{K}_{\mathrm{OW}}$ is low and can be less than 1.0 , resulting in negative values of $\log K_{\text {Ow. }}$. In such cases, care should be taken when using correlations developed for more hydrophobic chemicals since partitioning into biota or organic carbon phases may be primarily into aqueous rather than organic media.

Details of experimental methods are described by Fujita et al. (1964), Leo et al. (1971), Hansch and Leo (1979), Rekker (1977), Chiou et al. (1977), Miller et al. (1984, 1985), Bowman and Sans (1983), Woodburn et al. (1984), Doucette and Andren (1987), and De Bruijn et al. (1989).

### 1.3.4 Henry's Law Constant

The Henry's law constant is essentially an air-water partition coefficient which can be determined by measurement of solute concentrations in both phases. This raises the difficulty of accurate analytical determination in two very different media which usually requires different techniques. Accordingly, effort has been devoted to devising techniques in which concentrations are measured in only one phase and the other concentration is deduced from a mass balance. These methods are generally more accurate. The principal difficulty arises with hydrophobic, low-volatility chemicals which can establish only very small concentrations in both phases.

Henry's law constant can be regarded as a ratio of vapor pressure to solubility, thus it is subject to the same effects that electrolytes have on solubility. Temperature affects both properties. Some methods are as follows:
a. Volatility measurement of dilute aqueous solutions (Butler et al. 1935, Burnett 1963, Buttery et al. 1969);
b. Multiple equilibration method (McAuliffe 1971, Munz and Roberts 1987);
c. Equilibrium batch stripping (Mackay et al. 1979, Dunnivant et al. 1988, Betterton and Hoffmann 1988, Zhou and Mopper 1990);
d. GC-determined distribution coefficients (Leighton and Calo 1981);
e. GC analysis of both air/water phases (Vejrosta et al. 1982, Jönsson et al. 1982);
f. EPICS (Equilibrium Partitioning In Closed Systems) method (Lincoff and Gossett 1984, Gossett 1987, Ashworth et al. 1988);
g. Wetted-wall column (Fendinger and Glotfelty 1988, 1989, 1990);
h. Headspace analyses (Hussam and Carr 1985);
i. Calculation from vapor pressure and solubility (Mackay and Shiu 1981);
j. GC retention volume/time determined activity coefficient at infinite dilution $\gamma^{\infty}$ (Karger et al. 1971a,b, Sugiyama et al. 1975, Tse et al. 1992).

When using vapor pressure and solubility data, it is essential to ensure that both properties apply to the same chemical phase, i.e., both are of the liquid, or of the solid. Occasionally, a solubility is of a solid while a vapor pressure is extrapolated from higher temperature liquid phase data.

As was discussed earlier under solubility, for miscible chemicals it is necessary to determine the Henry's law constant directly, since solubilities are not measurable.

### 1.3.5 Octanol-Air Partition Coefficient Koa

As was discussed earlier the octanol-air partition coefficient is increasingly used as a descriptor of partitioning between the atmosphere and organic phases in soils and vegetation. A generator column technique is generally used in which an inert gas is flowed through a column containing a substance dissolved in octanol. The concentration in the equilibrated gas leaving the column is then measured (Harner and Mackay 1995). More recent methods have been described by Harner and Bidleman (1996) and Shoeib and Harner (2002). Su et al (2002) have described a GC retention time method.

### 1.4 QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIPS (QSPRs)

### 1.4.1 Objectives of QSPRs

Because of the large number of chemicals of actual and potential concern, the difficulties and cost of experimental determinations, and scientific interest in elucidating the fundamental molecular determinants of physical-chemical properties, considerable effort has been devoted to generating quantitative structure-property relationships (QSPRs). This concept of structure-property relationships or structure-activity relationships (QSARs) is based on observations of linear free-energy relationships, and usually takes the form of a plot or regression of the property of interest as a function of an appropriate molecular descriptor which can be calculated using only a knowledge of molecular structure or a readily accessible molecular property.

Such relationships have been applied to solubility, vapor pressure, $\mathrm{K}_{\mathrm{ow}}, \mathrm{K}_{\mathrm{AW}}, \mathrm{K}_{\mathrm{OA}}$, Henry's law constant, reactivities, bioconcentration data and several other environmentally relevant partition coefficients. Of particular value are relationships involving various manifestations of toxicity, but these are beyond the scope of this handbook. These relationships are valuable because they permit values to be checked for "reasonableness" and (with some caution) interpolation is possible to estimate undetermined values. They may be used (with extreme caution!) for extrapolation.

A large number of descriptors have been, and are being, proposed and tested. Dearden (1990) and the compilations by Karcher and Devillers (1990) and Hermens and Opperhuizen (1991) give comprehensive accounts of descriptors and their applications.

A valuable source of up-to-date information is the proceedings of the biennial QSAR conferences. The QSAR 2002 conference proceedings have been edited by Breton et al. (2003). A set of critical reviews has been edited by Walker (2003). Of particular note is the collection of estimation methods developed by the Syracuse Research Corporation with US EPA support and available on the internet at www.syrres.com under "estimation methods."

Among the most commonly used molecular descriptors are molecular weight and volume, the number of specific atoms (e.g., carbon or chlorine), surface areas (which may be defined in various ways), refractivity, parachor, steric parameters, connectivities and various topological parameters. Several quantum chemical parameters can be calculated from molecular orbital calculations including charge, electron density and superdelocalizability. It is likely that existing and new descriptors will continue to be tested, and that eventually a generally preferred set of readily accessible parameters will be adopted for routine use for correlating purposes.

From the viewpoint of developing quantitative correlations it is desirable to seek a linear relationship between descriptor and property, but a nonlinear or curvilinear relationship is adequate for illustrating relationships and interpolating purposes. In this handbook we have elected to use the simple descriptor of molar volume at the normal boiling point as estimated by the Le Bas method (Reid et al. 1987). This parameter is very easily calculated and proves to be adequate for the present purposes of plotting property versus relationship without seeking linearity.

The Le Bas method is based on a summation of atomic volumes with adjustment for the volume decrease arising from ring formation. The full method is described by Reid et al. (1987), but for the purposes of this compilation, the volumes and rules as listed in Table 1.3.1 are used.

Example: The experimental molar volume of chlorobenzene $115 \mathrm{~cm}^{3} / \mathrm{mol}$ (Reid et al. 1987). From the above rules, the Le Bas molar volume for chlorobenzene $\left(\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{Cl}\right)$ is:

$$
\mathrm{V}=6 \times 14.8+5 \times 3.7+24.6-15=117 \mathrm{~cm}^{3} / \mathrm{mol}
$$

Accordingly, plots are presented at the end of each chapter for solubility, vapor pressure, $\mathrm{K}_{\mathrm{ow}}$, and Henry's law constant versus Le Bas molar volume.

TABLE 1.3.1
Le Bas molar volume

|  | increment, $\mathbf{c m}^{3} / \mathbf{m o l}$ |
| :--- | :---: |
| Carbon | 14.8 |
| Hydrogen | 3.7 |
| Oxygen | 7.4 |
| $\quad$ In methyl esters and ethers | 9.1 |
| In ethyl esters and ethers | 9.9 |
| $\quad$ Join to S, P, or N | 8.3 |
| Nitrogen |  |
| $\quad$ Doubly bonded | 15.6 |
| $\quad$ In primary amines | 10.5 |
| $\quad$ In secondary amines | 12.0 |
| Bromine | 27.0 |
| Chlorine | 24.6 |
| Fluorine | 8.7 |
| Iodine | 37.0 |
| Sulfur | 25.6 |
| Rings |  |
| $\quad$ Three-membered | -6.0 |
| Four-membered | -8.5 |
| Five-membered | -11.5 |
| Six-membered | -15.0 |
| Naphthalene | -30.0 |
| Anthracene | -47.5 |

As was discussed earlier in Section 1.2.8 a complication arises in that two of these properties (solubility and vapor pressure) are dependent on whether the solute is in the liquid or solid state. Solid solutes have lower solubilities and vapor pressures than they would have if they had been liquids. The ratio of the (actual) solid to the (hypothetical supercooled) liquid solubility or vapor pressure is termed the fugacity ratio F and can be estimated from the melting point and the entropy of fusion. This "correction" eliminates the effect of melting point, which depends on the stability of the solid crystalline phase, which in turn is a function of molecular symmetry and other factors. For solid solutes, the correct property to plot is the calculated or extrapolated supercooled liquid solubility. This is calculated in this handbook using where possible a measured entropy of fusion, or in the absence of such data the Walden's Rule relationship suggested by Yalkowsky (1979) which implies an entropy of fusion of $56 \mathrm{~J} / \mathrm{mol} \cdot \mathrm{K}$ or $13.5 \mathrm{cal} / \mathrm{mol} \cdot \mathrm{K}$ (e.u.)

$$
F=C_{\mathrm{S}}^{\mathrm{S}} / C_{\mathrm{L}}^{\mathrm{S}}=P_{\mathrm{S}}^{\mathrm{S}} / P_{\mathrm{L}}^{\mathrm{S}}=\exp \left\{6.79\left(1-T_{\mathrm{M}} / T\right)\right\}
$$

where $C^{\mathrm{S}}$ is solubility, $P^{\mathrm{S}}$ is vapor pressure, subscripts S and L refer to solid and liquid phases, $\mathrm{T}_{\mathrm{M}}$ is melting point and $T$ is the system temperature, both in absolute ( K ) units. The fugacity ratio is given in the data tables at $25^{\circ} \mathrm{C}$, the usual temperature at which physical-chemical property data are reported. For liquids, the fugacity ratio is 1.0 .

The usual approach is to compile data for the property in question for a series of structurally similar molecules and plot the logarithm of this property versus molecular descriptors, on a trial-and-error basis seeking the descriptor which best characterizes the variation in the property. It may be appropriate to use a training set to obtain a relationship and test this relationship on another set. Generally a set of at least ten data points is necessary before a reliable QSPR can be developed.

### 1.4.2 Examples of QSARs and QSPRs

There is a continuing effort to extend the long-established concept of quantitative-structure-activity-relationships (QSARs) to quantitative-structure-property relationships (QSPRs) to compute all relevant environmental physicalchemical properties (such as aqueous solubility, vapor pressure, octanol-water partition coefficient, Henry's law constant, bioconcentration factor (BCF), sorption coefficient and environmental reaction rate constants from molecular structure).

Examples are Burkhard (1984) and Burkhard et al. (1985a), who calculated solubility, vapor pressure, Henry's law constant, $K_{\mathrm{OW}}$ and $K_{\mathrm{OC}}$ for all PCB congeners. Hawker and Connell (1988) also calculated $\log K_{\mathrm{Ow}}$; Abramowitz and Yalkowsky (1990) calculated melting point and solubility for all PCB congeners based on the correlation with total surface area (planar TSAs). Doucette and Andren (1988b) used six molecular descriptors to compute the $K_{\text {ow }}$ of some chlorobenzenes, PCBs and PCDDs. Mailhot and Peters (1988) employed seven molecular descriptors to compute physical-chemical properties of some 300 compounds. Isnard and Lambert $(1988,1989)$ correlated solubility, $K_{\text {ow }}$ and BCF for a large number of organic chemicals. Nirmalakhandan and Speece (1988a,b, 1989) used molecular connectivity indices to predict aqueous solubility and Henry's law constants for 300 compounds over 12 logarithmic units in solubility. Kamlet and co-workers $(1986,1987,1988)$ have developed the "solvatochromic" parameters with the intrinsic molar volume to predict solubility, $\log K_{\text {ow }}$ and toxicity of organic chemicals. Warne et al. (1990) correlated solubility and $K_{\text {Ow }}$ for lipophilic organic compounds with 39 molecular descriptors and physical-chemical properties. Atkinson (1987, 1988) has used the structure-activity relationship (SAR) to estimate gas-phase reaction rate constants of hydroxyl radicals for organic chemicals. Mabey et al. (1984) have reviewed the estimation methods from SAR correlation for reaction rate constants and physical-chemical properties in environmental fate assessment. Other correlations are reviewed by Lyman et al. (1982) and Yalkowsky and Banerjee (1992). As Dearden (1990) has pointed out, "new parameters are continually being devised and tested, although the necessity of that may be questioned, given the vast number already available." It must be emphasized, however, that regardless of how accurate these predicted or estimated properties are claimed to be, ultimately they have to be confirmed or verified by experimental measurement.

A fundamental problem encountered in these correlations is the mismatch between the accuracy of experimental data and the molecular descriptors which can be calculated with relatively high precision, usually within a few percent. The accuracy may not always be high, but for correlation purposes precision is more important than accuracy. The precision and accuracy of the experimental data are often poor, frequently ranging over a factor of two or more. Certain isomers may yield identical descriptors, but have different properties. There is thus an inherent limit to the applicability of QSPRs imposed by the quality of the experimental data, and further efforts to improve descriptors, while interesting and potentially useful, may be unlikely to yield demonstrably improved QSPRs.

One of the most useful and accessible set of QSARs is that developed primarily by Howard and Meylan at the Syracuse Research Corporation, NY. These estimation methods are available as the EPISuite set from their website at www.syrres.com.

For correlation of solubility, the correct thermodynamic quantities for correlation are the activity coefficient $\gamma$, or the excess Gibbs free energy $\Delta \mathrm{G}$, as discussed by Pierotti et al. (1959) and Tsonopoulos and Prausnitz (1971). Examples of such correlations are given below.

1. Carbon number or carbon plus chlorine number (Tsonopoulos and Prausnitz 1971, Mackay and Shiu 1977);
2. Molar volume $\mathrm{cm}^{3} / \mathrm{mol}$
a. Liquid molar volume - from density (McAuliffe 1966, Lande and Banerjee 1981, Chiou et al. 1982, Abernethy et al. 1988, Wang et al. 1992);
b. Molar volume by additive group contribution method, e.g., Le Bas method, Schroeder method (Reid et al. 1987, Miller et al. 1985);
c. Intrinsic molar volume, $\mathrm{V}_{\mathrm{I}}, \mathrm{cm}^{3} / \mathrm{mol}$ - from van der Waals radius with solvatochromic parameters $\alpha$ and $\beta$ (Leahy 1986, Kamlet et al. 1987, 1988);
d. Characteristic molecular volume, $\mathrm{m}^{3} / \mathrm{mol}$ (McGowan and Mellors 1986);
3. Group contribution method (Irmann 1965, Korenman et al. 1971, Polak and Lu 1973, Klopman et al. 1992);
4. Molecular volume - $\AA^{3} /$ molecule (cubic Angstrom per molecule)
a. van der Waals volume (Bondi 1964);
b. Total molecular volume (TMV) (Pearlman et al. 1984, Pearlman 1986);
5. Total surface area (TSA) - $\AA^{2} /$ molecule (Hermann 1971, Amidon et al. 1975, Yalkowsky and Valvani 1976, Yalkowsky et al. 1979, Iwase et al. 1985, Pearlman 1986, Andren et al. 1987, Hawker and Connell 1988, Dunnivant et al. 1992);
6. Molecular connectivity indices (MCI) or $\chi$ (Kier and Hall 1976, Andren et al. 1987, Nirmalakhandan and Speece 1988b, 1989);
7. Boiling point (Almgren et al. 1979);
8. Melting point (Amidon and Williams 1982);
9. Melting point and TSA (Abramowitz and Yalkowsky 1990);
10. High-pressure liquid chromatography (HPLC) - retention data (Locke 1974, Whitehouse and Cooke 1982, Brodsky and Ballschmiter 1988);
11. Adsorbability index (AI) (Okouchi et al. 1992);
12. Fragment solubility constants (Wakita et al. 1986).

Several workers have explored the linear relationship between octanol-water partition coefficient and solubility as a means of estimating solubility.

Hansch et al. (1968) established the linear free-energy relationship between aqueous and octanol-water partition of organic liquid. Others, such as Tulp and Hutzinger (1978), Yalkowsky et al. (1979), Mackay et al. (1980), Banerjee et al. (1980), Chiou et al. (1982), Bowman and Sans (1983), Miller et al. (1985), Andren et al. (1987) and Doucette and Andren (1988b) have all presented similar but modified relationships.

The UNIFAC (UNIQUAC Functional Group Activity Coefficient) group contribution (Fredenslund et al. 1975, Kikic et al. 1980, Magnussen et al. 1981, Gmehling et al. 1982 and Hansen et al. 1991) is widely used for predicting the activity coefficient in nonelectrolyte liquid mixtures by using group-interaction parameters. This method has been used by Kabadi and Danner (1979), Banerjee (1985), Arbuckle (1983, 1986), Banerjee and Howard (1988) and Al-Sahhaf (1989) for predicting solubility (as a function of the infinite dilution activity coefficient, $\gamma^{\infty}$ ) in aqueous systems. Its performance is reviewed by Yalkowsky and Banerjee (1992).

HPLC retention time data have been used as a pseudo-molecular descriptor by Whitehouse and Cooke (1982), Hafkenscheid and Tomlinson (1981), Tomlinson and Hafkenscheid (1986) and Swann et al. (1983).

The octanol-water partition coefficient $K_{\mathrm{OW}}$ is widely used as a descriptor of hydrophobicity. Variation in $K_{\mathrm{OW}}$ is primarily attributable to variation in activity coefficient in the aqueous phase (Miller et al. 1985); thus, the same correlations used for solubility in water are applicable to $K_{\text {OW. }}$. Most widely used is the Hansch-Leo compilation of data (Leo et al. 1971, Hansch and Leo 1979) and related predictive methods. Examples of $K_{\text {OW }}$ correlations are:

1. Molecular descriptors
a. Molar volumes: Le Bas method; from density; intrinsic molar volume; characteristic molecular volume (Abernethy et al. 1988, Chiou 1985, Kamlet et al. 1988, McGowan and Mellors 1986);
b. TMV (De Bruijn and Hermens 1990);
c. TSA (Yalkowsky et al. 1979, 1983, Pearlman 1980, 1986, Pearlman et al. 1984, Hawker and Connell 1988);
d. Molecular connectivity indices (Doucette and Andren 1988b);
e. Molecular weight (Doucette and Andren 1988b).
2. Group contribution methods
a. $\pi$-constant or hydrophobic substituent method (Hansch et al. 1968, Hansch and Leo 1979, Doucette and Andren 1988b);
b. Fragment constants or f-constant (Rekker 1977, Yalkowsky et al. 1983);
c. Hansch and Leo's f-constant (Hansch and Leo 1979; Doucette and Andren 1988b).
3. From solubility - $K_{\text {OW }}$ relationship
4. HPLC retention data
a. HPLC-k' capacity factor (Könemann et al. 1979, McDuffie 1981);
b. HPLC-RT retention time (Veith et al. 1979, Rapaport and Eisenreich 1984, Doucette and Andren 1988b);
c. HPLC-RV retention volume (Garst 1984);
d. HPLC-RT/MS HPLC retention time with mass spectrometry (Burkhard et al. 1985c).
5. Reversed-phase thin-layer chromatography (TLC) (Ellgehausen et al. 1981, Bruggeman et al. 1982).
6. Molar refractivity (Yoshida et al. 1983).
7. Combination of HPLC retention data and molecular connectivity indices (Finizio et al. 1994).
8. Molecular orbital methods (Reddy and Locke 1994).

As with solubility and octanol-water partition coefficient, vapor pressure can be estimated with a variety of correlations as discussed in detail by Burkhard et al. (1985a) and summarized as follows:

1. Interpolation or extrapolation from equation for correlating temperature relationships, e.g., the ClausiusClapeyron, Antoine equations (Burkhard et al. 1985a);
2. Carbon or chlorine numbers (Mackay et al. 1980, Shiu and Mackay 1986);
3. Le Bas molar volume (Shiu et al. 1987, 1988);
4. Boiling point $T_{\mathrm{B}}$ and heat of vaporization $\Delta H_{\mathrm{v}}$ (Mackay et al. 1982);
5. Group contribution method (Macknick and Prausnitz 1979);
6. UNIFAC group contribution method (Jensen et al. 1981, Yair and Fredenslund 1983, Burkhard et al. 1985a, Banerjee et al.1990);
7. Molecular weight and Gibbs' free energy of vaporization $\Delta G_{\mathrm{v}}$ (Burkhard et al. 1985a);
8. TSA and $\Delta G_{\mathrm{v}}$ (Amidon and Anik 1981, Burkhard et al. 1985a, Hawker 1989);
9. Molecular connectivity indices (Kier and Hall 1976, 1986, Burkhard et al. 1985a);
10. Melting point $T_{\mathrm{M}}$ and GC retention index (Bidleman 1984, Burkhard et al. 1985a);
11. Solvatochromic parameters and intrinsic molar volume (Banerjee et al. 1990).

As described earlier, Henry's law constants can be calculated from the ratio of vapor pressure and aqueous solubility. Henry's law constants do not show a simple linear pattern as solubility, $\mathrm{K}_{\mathrm{Ow}}$ or vapor pressure when plotted against simple molecular descriptors, such as numbers of chlorine or Le Bas molar volume, e.g., PCBs (Burkhard et al. 1985b), pesticides (Suntio et al. 1988), and chlorinated dioxins (Shiu et al. 1988). Henry's law constants can be estimated from:

1. UNIFAC-derived infinite dilution activity coefficients (Arbuckle 1983);
2. Group contribution and bond contribution methods (Hine and Mookerjee 1975, Meylan and Howard 1991);
3. Molecular connectivity indices (Nirmalakhandan and Speece 1988b, Sabljic and Güsten 1989, Dunnivant et al. 1992);
4. Total surface area - planar TSA (Hawker 1989);
5. Critical reviews by Mackay and Shiu 1981, Shiu and Mackay 1986 and Suntio et al. 1988.

For water-miscible compounds the use of aqueous solubility data is obviously impossible.

## Bioconcentration Factors:

1. Correlation with $K_{\text {Ow }}$ (Neely et al. 1974, Könemann and van Leeuwen 1980, Veith et al. 1980, Chiou et al. 1977, Mackay 1982, Briggs 1981, Garten and Trabalka 1983, Davies and Dobbs 1984, Zaroogian et al. 1985, Oliver and Niimi 1988, Isnard and Lambert 1988);
2. Correlation with solubility (Kenaga 1980, Kenaga and Goring 1980, Briggs 1981, Garten and Trabalka 1983, Davies and Dobbs 1984, Isnard and Lambert 1988);
3. Correlation with $K_{\mathrm{OC}}$ (Kenaga 1980, Kenaga and Goring 1980, Briggs 1981);
4. Calculation with HPLC retention data (Swann et al. 1983);
5. Calculation with solvatochromic parameters (Hawker 1989, 1990b).

## Sorption Coefficients:

1. Correlation with $K_{\mathrm{OW}}$ (Karickhoff et al. 1979, Schwarzenbach and Westall 1981, Mackay 1982, Oliver 1984);
2. Correlation with solubility (Karickhoff et al. 1979);
3. Molecular connectivity indices (Gerstl and Helling 1984; Sabljic 1984, 1987, Bahnick and Doucette 1988, Sabljic et al. 1989, Meylan et al. 1992);
4. Estimation from molecular connectivity index/fragment contribution method (Meylan et al. 1992, Lohninger 1994);
5. From HPLC retention data (Swann et al. 1983, Szabo et al. 1990).
6. Molecular orbital method (Reddy and Locke 1994).

## Octanol-Air Partition coefficient.

The molecular descriptors used for $\mathrm{K}_{\mathrm{OW}}$, solubility in water and vapor pressure can potentially be applied to $\mathrm{K}_{\mathrm{OA}}$.

### 1.5 MASS BALANCE MODELS OF CHEMICAL FATE

### 1.5.1 Evaluative Environmental Calculations

When conducting assessments of how a chemical is likely to behave in the environment and especially how different chemicals behave in the same environment, there is incentive to standardize the evaluations using "evaluative" environmental models. The nature of these calculations has been described in a series of papers, notably Mackay (1979),

Paterson and Mackay (1985), Mackay and Paterson (1990, 1991), and a recent text (Mackay 2001). Only the salient features are presented here. Three evaluations are completed for each chemical, namely the Level I, II and III fugacity calculations. These calculations can also be done in concentration format instead of fugacity, but for this type of evaluation the fugacity approach is simpler and more instructive. The mass balance models of the types described below can be downloaded for the web site www.trentu.ca/cemc

### 1.5.2 Level I Fugacity Calculations

The Level I calculation describes how a given amount of chemical partitions at equilibrium between six media: air, water, soil, bottom sediment, suspended sediment and fish. No account is taken of reactivity. Whereas most early evaluative environments have treated a one square kilometre region with about $70 \%$ water surface (simulating the global proportion of ocean surface), it has become apparent that a more useful approach is to treat a larger, principally terrestrial area similar to a jurisdictional region such as a US state. The area selected is $100,000 \mathrm{~km}^{2}$ or $10^{11} \mathrm{~m}^{2}$, which is about the area of Ohio, Greece or England. This environment was used in previous editions of this Handbook and is identical to the EQC or Equilibrium Criterion model described by Mackay et al. (1996).

The atmospheric height is selected as an arbitrary 1000 m reflecting that region of the troposphere which is most affected by local air emissions. A water surface area of $10 \%$ or $10,000 \mathrm{~km}^{2}$ is used, with a water depth of 20 m . The water volume is thus $2 \times 10^{11} \mathrm{~m}^{3}$. The soil is viewed as being well mixed to a depth of 10 cm and is considered to be $2 \%$ organic carbon. It has a volume of $9 \times 10^{9} \mathrm{~m}^{3}$. The bottom sediment has the same area as the water, a depth of 1 cm and an organic carbon content of $4 \%$. It thus has a volume of $10^{8} \mathrm{~m}^{3}$.

For the Level I calculation both the soil and sediment are treated as simple solid phases with the above volumes, i.e., the presence of air or water in the pores of these phases is ignored.

Two other phases are included for interest. Suspended matter in water is often an important medium when compared in sorbing capacity to that of water. It is treated as having $20 \%$ organic carbon and being present at a volume fraction in the water of $5 \times 10^{-6}$, i.e., it is about 5 to $10 \mathrm{mg} / \mathrm{L}$. The volume is thus $10^{6} \mathrm{~m}^{3}$. Fish is also included at an entirely arbitrary volume fraction of $10^{-6}$ and are assumed to contain $5 \%$ lipid, equivalent in sorbing capacity to octanol. The volume is thus $2 \times 10^{5} \mathrm{~m}^{3}$. These two phases are small in volume and rarely contain an appreciable fraction of the chemical present, but it is in these phases that the highest concentration of chemical often exists.

Another phase which is introduced later in the Level III model is aerosol particles with a volume fraction in air of $2 \times 10^{-11}$, i.e., approximately $30 \mu \mathrm{~g} / \mathrm{m}^{3}$. Although negligible in volume, an appreciable fraction of the chemical present in the air phase may be associated with aerosols. Aerosols are not treated in Level I or II calculations because their capacity for the chemical at equilibrium is usually negligible when compared with soil.

These dimensions and properties are summarized in Tables 1.5.1 and 1.5.2. The user is encouraged to modify these dimensions to reflect conditions in a specific area of interest.

The amount of chemical introduced in the Level I calculation is an arbitrary $100,000 \mathrm{~kg}$ or 100 tonnes. If dispersed entirely in the air, this amount yields a concentration of $1 \mu \mathrm{~g} / \mathrm{m}^{3}$ which is not unusual for ubiquitous contaminants such as hydrocarbons. If dispersed entirely in the water, the concentration is a higher $500 \mu \mathrm{~g} / \mathrm{m}^{3}$ or $500 \mathrm{ng} / \mathrm{L}$, which again is reasonable for a well-used chemical of commerce. The corresponding value in soil is about $0.0046 \mu \mathrm{~g} / \mathrm{g}$. Clearly for restricted chemicals such as PCBs, this amount is too large, but it is preferable to adopt a common evaluative amount

## TABLE 1.5.1

## Compartment dimensions and properties for Levels I and II calculations

| Compartment | Air | Water | Soil | Sediment | Suspended <br> sediment | Fish |
| :--- | :--- | :--- | :--- | :--- | :--- | :---: |
| Volume, $\mathrm{V}\left(\mathrm{m}^{3}\right)$ | $10^{14}$ | $2 \times 10^{11}$ | $9 \times 10^{9}$ | $10^{8}$ | $10^{6}$ | $2 \times 10^{5}$ |
| Depth, $\mathrm{h}(\mathrm{m})$ | 1000 | 20 | 0.1 | 0.01 | - | - |
| Area, $\mathrm{A}\left(\mathrm{m}^{2}\right)$ | $100 \times 10^{9}$ | $10 \times 10^{9}$ | $90 \times 10^{9}$ | $10 \times 10^{9}$ | - | - |
| Fraction OC | - | - | 0.02 | 0.04 | 0.2 | - |
| Density, $\rho\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ | 1.2 | 1000 | 2400 | 2400 | 1500 | 1000 |
| Adv. Residence | 100 | 1000 | - | 50,000 | - | - |
| Time, $\mathrm{t}($ hours $)$ |  |  |  |  | 2000 | - |
| Adv. flow, $\mathrm{G}\left(\mathrm{m}^{3} / \mathrm{h}\right)$ | $10^{12}$ | $2 \times 10^{8}$ | - |  | - |  |

TABLE 1.5.2
Bulk compartment dimensions and volume fractions (v) for Level III calculations

## Compartment

| Air | Total volume <br> Air phase <br> Water |
| :--- | :--- |
|  | Aerosol phase <br> Total volume <br> Water phase |
|  | Suspended sediment phase <br> Soil |
|  | Fish phase <br> Total volume <br> Air phase |
|  | Water phase <br> Sediment |
|  | Solid phase <br> Total volume <br> Water phase |
|  | Solid phase |

## Volume

$$
\begin{aligned}
& 10^{14} \mathrm{~m}^{3}(\text { as above }) \\
& 10^{14} \mathrm{~m}^{3} \\
& 2000 \mathrm{~m}^{3}\left(\mathrm{v}=2 \times 10^{-11}\right) \\
& 2 \times 10^{11} \mathrm{~m}^{3} \\
& 2 \times 10^{11} \mathrm{~m}^{3}(\text { as above }) \\
& 10^{6} \mathrm{~m}^{3}\left(\mathrm{v}=5 \times 10^{-6}\right) \\
& 2 \times 10^{5} \mathrm{~m}^{3}\left(\mathrm{v}=1 \times 10^{-6}\right) \\
& 18 \times 10^{9} \mathrm{~m}^{3} \\
& 3.6 \times 10^{9} \mathrm{~m}^{3}(\mathrm{v}=0.2) \\
& 5.4 \times 10^{9} \mathrm{~m}^{3}(\mathrm{v}=0.3) \\
& 9.0 \times 10^{9} \mathrm{~m}^{3}(\mathrm{v}=0.5)(\text { as above }) \\
& 500 \times 10^{6} \mathrm{~m}^{3} \\
& 400 \times 10^{6} \mathrm{~m}^{3}(\mathrm{v}=0.8) \\
& 100 \times 10^{6} \mathrm{~m}^{3}(\mathrm{v}=0.2)(\text { as above })
\end{aligned}
$$

TABLE 1.5.3
Equations for phase Z values used in Levels I, II and bulk phase values used in Level III

Compartment
Air
Water
Soil
Sediment
Suspended Sediment
Fish
Aerosol
where
$Z$ values
$\mathrm{Z}_{1}=1 / \mathrm{RT}$
$\mathrm{Z}_{2}=1 / \mathrm{H}=\mathrm{C}^{\mathrm{S}} / \mathrm{P}^{\mathrm{S}}$
$\mathrm{Z}_{3}=\mathrm{Z}_{2} \cdot \rho_{3} \cdot \phi_{3} \cdot \mathrm{~K}_{\mathrm{OC}} / 1000$
$\mathrm{Z}_{4}=\mathrm{Z}_{2} \cdot \rho_{4} \cdot \phi_{4} \cdot \mathrm{~K}_{\mathrm{OC}} / 1000$
$\mathrm{Z}_{5}=\mathrm{Z}_{2} \cdot \rho_{5} \cdot \phi_{5} \cdot \mathrm{~K}_{\mathrm{OC}} / 1000$
$\mathrm{Z}_{6}=\mathrm{Z}_{2} \cdot \rho_{6} \cdot \mathrm{~L} \cdot \mathrm{~K}_{\text {ow }} / 1000$
$\mathrm{Z}_{7}=\mathrm{Z}_{1} \cdot 6 \times 10^{6} / \mathrm{P}_{\mathrm{L}}^{\mathrm{S}}$ or $0.1 \mathrm{Z}_{1} \mathrm{~K}_{\mathrm{OA}}$
$\mathrm{R}=$ gas constant ( $8.314 \mathrm{~J} / \mathrm{mol} \cdot \mathrm{K}$ )
$\mathrm{T}=$ absolute temperature ( K )
$\mathrm{C}^{\text {S }}=$ solubility in water $\left(\mathrm{mol} / \mathrm{m}^{3}\right)$
$\mathrm{P}^{\mathrm{S}}=$ vapor pressure $(\mathrm{Pa})$
$\mathrm{H}=$ Henry's law constant $\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)$
$\mathrm{P}_{\mathrm{L}}^{\mathrm{S}}=$ liquid vapor pressure $(\mathrm{Pa})$
$\mathrm{K}_{\mathrm{OA}}=$ octanol-air partition coefficient
$\mathrm{K}_{\mathrm{Ow}}=$ octanol-water partition coefficient
$\rho_{\mathrm{i}}=$ density of phase $\mathrm{i}\left(\mathrm{kg} / \mathrm{m}^{3}\right)$
$\phi_{i}=$ mass fraction organic-carbon in phase $i(\mathrm{~g} / \mathrm{g})$
$\mathrm{L}=$ lipid content of fish

Note for solids $\mathrm{P}_{\mathrm{L}}^{\mathrm{S}}=\mathrm{P}_{\mathrm{S}}^{\mathrm{S}} / \exp \left\{6.79\left(1-\mathrm{T}_{\mathrm{M}} / \mathrm{T}\right)\right\}$, where $\mathrm{T}_{\mathrm{M}}$ is melting point $(\mathrm{K})$ of the solute and T is 298 K . An experimental entropy of fusion should be used if available.
for all substances. No significance should, of course, be attached to the absolute values of the concentrations which are deduced from this arbitrary amount. Only the relative values have significance.

The Level I calculation proceeds by deducing the fugacity capacities or Z values for each medium (see Table 1.5.3), following the procedures described by Mackay (2001). These working equations show the necessity of having data on molecular mass, water solubility, vapor pressure, and octanol-water partition coefficient. The fugacity $f(\mathrm{~Pa})$ common to all media is deduced as

$$
\mathrm{f}=\mathrm{M} / \Sigma \mathrm{V}_{\mathrm{i}} \mathrm{Z}_{\mathrm{i}}
$$

where M is the total amount of chemical (mol), $\mathrm{V}_{\mathrm{i}}$ is the medium volume $\left(\mathrm{m}^{3}\right)$ and $\mathrm{Z}_{\mathrm{i}}$ is the corresponding fugacity capacity for the chemical in each medium. It is noteworthy that $Z$ values contain all the necessary partition information. The partition coefficient $K_{12}$ is simply the ratio of $Z$ values, i.e., $Z_{1} / Z_{2}$. Definition of the $Z$ values starts in the air compartment then proceeds to other compartments using the appropriate partition coefficients.

The molar concentration $\mathrm{C}\left(\mathrm{mol} / \mathrm{m}^{3}\right)$ can then be deduced as $\mathrm{Zf} \mathrm{mol} / \mathrm{m}^{3}$ or as $\mathrm{WZf} \mathrm{g} / \mathrm{m}^{3}$ or $1000 \mathrm{WZf} / \rho \mu \mathrm{g} / \mathrm{g}$, where $\rho$ is the phase density $\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ and W is the molecular mass $(\mathrm{g} / \mathrm{mol})$. The amount $\mathrm{m}_{\mathrm{i}}$ in each medium is $\mathrm{C}_{\mathrm{i}} \mathrm{V}_{\mathrm{i}}$ mol, and the total in all media is M mol. The information obtained from this calculation includes the concentrations, amounts and distribution.

Note that this simple treatment assumes that the soil and sediment phases are entirely solid, i.e., there are no air or water phases present to "dilute" the solids. Later in the Level III calculation these phases and aerosols are included (see Table 1.5.4).

## Correction for Dissociation

As discussed earlier in Section 1.2.4, for dissociating or ionizing organic chemicals in aqueous solution, it is necessary to consider the effect of pH and thus the degree of dissociation, and to calculate the concentrations of both ionic and non-ionic species. The EQC model does not address dissociation.

The Z values are calculated using the conventional equations at the pH of the experimental data (i.e., the system $\mathrm{pH})$. The total Z value in water is then separated into its ionic and non-ionic contributions, i.e., fractions of $\mathrm{I} /(\mathrm{I}+1)$ and $\mathrm{l} /(\mathrm{I}+1)$. The Z value for the non-ionic form in water is assumed to apply at all pHs i.e., including the environmental pH , but an additional and possibly different ionic Z value in water is deduced at the environmental pH using I calculated at that pH . The total Z values in water are then calculated. Z values in other media are unaffected.

The calculation is illustrated in Table 1.5 .5 for pentachlorophenol. The experimental aqueous solubility is $14.0 \mathrm{~g} / \mathrm{m}^{3}$ at a pH of 5.1. The environmental pH is 7 . Higher environmental pH increases the extent of dissociation, thus increasing the Z value in water, increasing the apparent solubility, decreasing the apparent $\mathrm{K}_{\mathrm{Ow}}$ and Henry's law constant and the air-water partition coefficient, and decreasing the soil-water partition coefficient.

Note: At pH of 5.1, $\mathrm{K}_{\mathrm{ow}}$ is 112200 and is the ratio of concentration in octanol to total concentration in water comprising fractions $1 /(1+\mathrm{I})$ or $1 /(1+2.29)$ or 0.304 of neutral and 0.696 of ionic species. $\mathrm{K}_{\mathrm{ow}}$ is thus $112200 / 0.304$ or 369000 for the neutral species and zero for the ionic species. For the neutral species $\mathrm{K}_{\mathrm{OC}}$ is assumed to be $0.41 \cdot \mathrm{~K}_{\mathrm{Ow}}$ or 151300 , thus $\mathrm{K}_{\mathrm{P}}$ is $151300 \times 0.02 \mathrm{~L} / \mathrm{kg}$, i.e., 3027 for a soil of $2 \%$ organic carbon. $\mathrm{K}_{\mathrm{Sw}}$ is thus $3027 \times 2.4$ where 2.4 is the solid density $(\mathrm{kg} / \mathrm{L})$ or $7265 . \mathrm{Z}_{\mathrm{S}}$ for the neutral species is thus $7265 \times \mathrm{Z}_{\mathrm{w}}$ or 27970 . At pH of 7 , the neutral species Z values are unaffected, but the Z value for water increases to 704 because of the greater extent of dissociation. $\mathrm{K}_{\mathrm{sw}}$ thus decreases to 27970/704 or 39.72.

TABLE 1.5.4
Bulk phase $Z$ values, $Z_{B i}$ deduced as $\Sigma v_{i} Z_{i}$, in which the coefficients, e.g., $2 \times 10^{-11}$, are the volume fractions $v_{i}$ of each pure phase as specified in Table 1.5.2

## Compartment

Air
Water
Soil
Sediment

## Bulk Z values

$\mathrm{Z}_{\mathrm{B} 1}=\mathrm{Z}_{1}+2 \times 10^{-11} \mathrm{Z}_{7}$
$\mathrm{Z}_{\mathrm{B} 2}=\mathrm{Z}_{2}+5 \times 10^{-6} \mathrm{Z}_{5}+1 \times 10^{-6} \mathrm{Z}_{6}$
$\mathrm{Z}_{\mathrm{B} 3}=0.2 \mathrm{Z}_{1}+0.3 \mathrm{Z}_{2}+0.5 \mathrm{Z}_{3}$
$\mathrm{Z}_{\mathrm{B} 4}=0.8 \mathrm{Z}_{2}+0.2 \mathrm{Z}_{4}$
(approximately $30 \mu \mathrm{~g} / \mathrm{m}^{3}$ aerosols
( 5 ppm solids, 1 ppm fish by volume)
( $20 \%$ air, $30 \%$ water, $50 \%$ solids)
(80\% water, $20 \%$ solids)

TABLE 1.5.5
Calculated Z values at different experimental and environmental pHs of pentachlorophenol. Z values at $25^{\circ} \mathrm{C}, \log \mathrm{K}_{\text {ow }}$ is $5.05, \mathrm{pK}_{\mathrm{a}} 4.74$, at data pH of 5.1 and environmental pH of 7.0 for air, water and soil of fraction organic carbon 0.02 and density of soil $2.4 \mathrm{~kg} / \mathrm{L}$

|  | At data $\mathbf{p H}$ of $5.1(I=2.29)$ |  | At environ. pH of $\mathbf{7}(\mathrm{I}=182)$ |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | Neutral | lonic | Total | Neutral | lonic | Total |
|  | $4.03 \times 10^{-4}$ | 0 | $4.03 \times 10^{-4}$ | $4.03 \times 10^{-4}$ | 0 | $4.03 \times 10^{-4}$ |
| Air | 3.85 | 8.82 | 12.67 | 3.85 | 700.4 | 704.2 |
| Water | 0 | 27970 | 27970 | 0 | 27970 |  |
| Soil solids | 27970 |  |  |  |  |  |

## TABLE 1.5.6

Calculated $Z_{w}$ values and some partition coefficients at different environmental pHs for pentachlorophenol (PCP), 2,4-dichlorophenol (2,4-DCP), 2,4,6-trichlorophenol (2,4,6-TCP) and p-cresol at $25^{\circ} \mathrm{C} . \mathrm{K}_{\mathrm{AW}}$ is the air-water partition coefficient and $\mathrm{K}_{\mathrm{SW}}$ is the soil-water partition coefficient

| $Z$ values in water |  |  |  |  |  | Partitioning properties |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| At pH | Neutral | Ionic | $\begin{aligned} & \text { Total } \\ & \mathrm{Z}_{\mathrm{w}} \end{aligned}$ | Fraction $x_{\mathrm{N}}$ | $\begin{gathered} \mathrm{S}_{\mathrm{T}} \\ \mathrm{~g} / \mathrm{m}^{3} \end{gathered}$ | $\mathrm{H}_{\mathrm{T}}$ <br> $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ | $\mathrm{K}_{\text {AW }}$ | $\mathrm{K}_{\text {SW }}$ |
| $P C P$ |  |  |  |  |  |  |  |  |
| 4 | 3.849 | 0.7004 | 4.549 | 0.846 | 16.55 | 0.224 | $8.9 \times 10^{-5}$ | 6147 |
| 6 | 3.849 | 70.04 | 73.89 | 0.052 | 268.8 | 0.0135 | $5.46 \times 10^{-6}$ | 378.5 |
| 7 | 3.849 | 700.4 | 704.2 | 0.0055 | 2562 | 0.00142 | $5.73 \times 10^{-7}$ | 39.7 |
| 2,4,6-TCP |  |  |  |  |  |  |  |  |
| 4 | 1.7677 | 0.0140 | 1.7817 | 0.992 | 434 | 0.5612 | $2.26 \times 10^{-4}$ | 105.2 |
| 6 | 1.7677 | 1.4041 | 3.1718 | 0.557 | 772 | 0.315 | $1.272 \times 10^{-4}$ | 59.09 |
| 7 | 1.7677 | 14.041 | 15.8088 | 0.118 | 3644 | 0.172 | $6.945 \times 10^{-5}$ | 11.86 |
| 2,4-DCP |  |  |  |  |  |  |  |  |
| 4 | 3.063 | 0.000386 | 3.063 | 1.0 | 6000 | 0.326 | 0.000132 | 31.24 |
| 6 | 3.063 | 0.0386 | 3.101 | 0.988 | 6073 | 0.322 | 0.000130 | 30.85 |
| 7 | 3.063 | 0.386 | 3.448 | 0.888 | 6760 | 0.290 | 0.000117 | 27.75 |
| p-Cresol |  |  |  |  |  |  |  |  |
| 4 | 11.97 | 0 | 11.948 | 1.0 | 22000 | 0.0836 | $3.37 \times 10^{-5}$ | 1.968 |
| 7 | 11.97 | 0.0066 | 11.975 | 1.0 | 22000 | 0.0836 | $3.35 \times 10^{-5}$ | 1.968 |

This is further demonstrated in Table 1.5 .6 which shows the effects of environmental pH on the partitioning behavior of 2,4-dichlorophenol ( $\mathrm{pK}_{\mathrm{a}}=7.90$, solubility of $6000 \mathrm{~g} / \mathrm{m}^{3}$ at pH of 5.1 and $\log \mathrm{K}_{\mathrm{ow}}=3.20$ ), 2,4,6-trichlorophenol $\left(\mathrm{pK}_{\mathrm{a}}=6.10\right.$, solubility of $430 \mathrm{~g} / \mathrm{m}^{3}$ at pH of 5.1 and $\left.\log \mathrm{K}_{\mathrm{ow}}=3.69\right)$, pentachlorophenol $\left(\mathrm{pK}_{\mathrm{a}}=4.74\right.$, solubility of $14.0 \mathrm{~g} / \mathrm{m}^{3}$ at pH of 5.1 and $\left.\log \mathrm{K}_{\mathrm{ow}}=5.05\right)$ and $p-\mathrm{cresol}\left(\mathrm{pK}_{\mathrm{a}}=10.26\right.$, a solubility of $22000 \mathrm{~g} / \mathrm{m}^{3}$ and $\left.\log \mathrm{K}_{\mathrm{ow}}=2.0\right)$ in the multimedia environment at $25^{\circ} \mathrm{C}$. For environmental pH from 4 to 7 , there is no significant effect for $p$-cresol (or for chemicals for which $\mathrm{pK}_{\mathrm{a}} \gg \mathrm{pH}$ ), very little effect for 2,4-dichlorophenol (and chemicals with $\mathrm{pK}_{\mathrm{a}}$ ranging between 7-10). There is some effect on 2,4,6-trichlorophenol (and chemicals with $\mathrm{pK}_{\mathrm{a}}$ of 6-7) and a large effect for pentachlorophenol.

A similar treatment can be applied to other dissociating compounds such as the carboxylic acids, nitrophenols. For bases such as amines the $\mathrm{pK}_{\mathrm{a}}$ is defined as ( $14-\mathrm{pK}_{\mathrm{b}}$ ), and the extent of dissociation is estimated as above.

### 1.5.3 Level II Fugacity Calculations

The Level II calculation simulates a situation in which a chemical is continuously discharged into the multimedia environment and achieves a steady-state and equilibrium condition, at which input and output rates are equal. The task is to deduce the rates of loss by reaction and advection and the prevailing concentrations and masses.

The reaction rate data developed for each chemical in the tables are used to select a reactivity class as described earlier, and hence a first-order rate constant for each medium. Often these rates are in considerable doubt; thus the quantities selected should be used with extreme caution because they may not be widely applicable. The rate constants $\mathrm{k}_{\mathrm{i}} \mathrm{h}^{-1}$ are used to calculate reaction $D$ values for each medium $D_{R i}$ as $V_{i} Z_{i} \mathrm{k}_{\mathrm{i}}$. The rate of reactive loss is then $\mathrm{D}_{\mathrm{Ri}} \mathrm{fmol} / \mathrm{h}$.

For advection, it is necessary to select flow rates. This is conveniently done in the form of advective residence times, $t$ in hour (h); thus the advection rate $G_{i}$ is $V_{i} / \mathrm{t} \mathrm{m}^{3} / \mathrm{h}$ for each medium. For air, a residence time of 100 hours is used (approximately 4 days), which is probably too long for the geographic area considered, but shorter residence times tend to cause air advective loss to be a dominant mechanism. For water, a figure of 1000 hours ( 42 days) is used, reflecting a mixture of rivers and lakes. For sediment burial (which is treated as an advective loss), a time of 50,000 hours or 5.7 years is used. Only for very persistent, hydrophobic chemicals is this process important. No advective loss from soil is included. The D value for loss by advection $\mathrm{D}_{\mathrm{Ai}}$ is $\mathrm{G}_{\mathrm{i}} \mathrm{Z}_{\mathrm{i}}$, and the rates are $\mathrm{D}_{\mathrm{Ai}} \mathrm{f} \mathrm{mol} / \mathrm{h}$.

There may thus be losses caused by both reaction and advection D values for the four primary media. These loss processes are not included for fish or suspended matter. At steady-state and equilibrium conditions, the input rate $\mathrm{E} \mathrm{mol} / \mathrm{h}$ can be equated to the sum of the output rates, from which the common fugacity can be calculated as follows

$$
\mathrm{E}=\mathrm{f} \cdot \Sigma \mathrm{D}_{\mathrm{Ai}}+\mathrm{f} \cdot \Sigma \mathrm{D}_{\mathrm{Ri}}
$$

thus,

$$
\mathrm{f}=\mathrm{E} /\left(\Sigma \mathrm{D}_{\mathrm{Ai}}+\Sigma \mathrm{D}_{\mathrm{Ri}}\right)
$$

The common assumed emission rate is $1000 \mathrm{~kg} / \mathrm{h}$ or 1 tonne $/ \mathrm{h}$. To achieve an amount equivalent to the 100 tonnes in the Level I calculation requires an overall residence time of 100 hours. Again, the concentrations and amounts $\mathrm{m}_{\mathrm{i}}$ and $\Sigma \mathrm{m}_{\mathrm{i}}$ or M can be deduced, as well as the reaction and advection rates. These rates obviously total to give the input rate E . Of particular interest are the relative rates of these loss processes, and the overall persistence or residence time, which is calculated as

$$
\mathrm{t}_{\mathrm{o}}=\mathrm{M} / \mathrm{E}
$$

where $M$ is the total amount present. It is also useful to calculate a reaction and an advection persistence $t_{R}$ and $t_{A}$ as

$$
\mathrm{t}_{\mathrm{R}}=\mathrm{M} / \Sigma \mathrm{D}_{\mathrm{Ri}} \mathrm{f} \quad \mathrm{t}_{\mathrm{A}}=\mathrm{M} / \Sigma \mathrm{D}_{\mathrm{Ai}} \mathrm{f}
$$

Obviously,

$$
1 / \mathrm{t}_{\mathrm{O}}=1 / \mathrm{t}_{\mathrm{R}}+1 / \mathrm{t}_{\mathrm{A}}
$$

These persistences indicate the likelihood of the chemical being lost by reaction as distinct from advection. The percentage distribution of chemical between phases is identical to that in Level I. A pie chart depicting the distribution of losses can be drawn.

### 1.5.4 Level III Fugacity Calculations

Whereas the Levels I and II calculations assume equilibrium to prevail between all media, this is recognized as being excessively simplistic and even misleading. In the interests of algebraic simplicity, only the four primary media are treated for this level. The task is to develop expressions for intermedia transport rates by the various diffusive and non-diffusive processes as described by Mackay (2001). This is done by selecting values for 12 intermedia transport velocity parameters which have dimensions of velocity ( $\mathrm{m} / \mathrm{h}$ or $\mathrm{m} / \mathrm{year}$ ), are designated as $\mathrm{U}_{\mathrm{i}} \mathrm{m} / \mathrm{h}$ and are applied to all chemicals. These parameters are used to calculate seven intermedia transport D values.

It is desirable to calculate new "bulk phase" Z values for the four primary media which include the contribution of dispersed phases within each medium as described by Mackay and Paterson (1991) and as listed earlier. The air is now treated as an air-aerosol mixture, water as water plus suspended particles and fish, soil as solids, air and water, and sediment as solids and porewater. The Z values thus differ from the Level I and Level II "pure phase" values. The necessity of introducing this complication arises from the fact that much of the intermedia transport of the chemicals occurs in association with the movement of chemical in these dispersed phases. To accommodate this change the same volumes of the soil solids and sediment solids are retained, but the total phase volumes are increased. These Level III volumes are also given in Table 1.5.2. The reaction and advection D values employ the generally smaller bulk phase Z values but the same residence times; thus the G values are increased and the D values are generally larger.

## Intermedia D Values

The justification for each intermedia $D$ value follows. It is noteworthy that, for example, air-to-water and water-to-air values differ because of the presence of one-way non-diffusive processes. A fuller description of the background to these calculations is given by Mackay (2001).

## 1. Air to Water $\left(D_{12}\right)$

Four processes are considered: diffusion (absorption), dissolution in rain of gaseous chemical, and wet and dry deposition of particle-associated chemical.

For diffusion, the conventional two-film approach is taken with water-side $\left(\mathrm{k}_{\mathrm{W}}\right)$ and air-side $\left(\mathrm{k}_{\mathrm{A}}\right)$ mass transfer coefficients ( $\mathrm{m} / \mathrm{h}$ ) being defined. Values of $0.05 \mathrm{~m} / \mathrm{h}$ for $\mathrm{k}_{\mathrm{W}}$ and $5 \mathrm{~m} / \mathrm{h}$ for $\mathrm{k}_{\mathrm{A}}$ are used. The absorption D value is then

$$
\mathrm{D}_{\mathrm{VW}}=1 /\left[1 /\left(\mathrm{k}_{\mathrm{A}} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{1}\right)+1 /\left(\mathrm{k}_{\mathrm{W}} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{2}\right)\right]
$$

where $A_{W}$ is the air-water area $\left(\mathrm{m}^{2}\right)$ and $\mathrm{Z}_{1}$ and $\mathrm{Z}_{2}$ are the pure air and water Z values. The velocities $\mathrm{k}_{\mathrm{A}}$ and $\mathrm{k}_{\mathrm{W}}$ are designated as $U_{1}$ and $U_{2}$.

For rain dissolution, a rainfall rate of $0.876 \mathrm{~m} /$ year is used, i.e., $U_{R}$ or $U_{3}$ is $10^{-4} \mathrm{~m} / \mathrm{h}$. The D value for rain dissolution $D_{R W}$ is then

$$
\mathrm{D}_{\mathrm{RW}}=\mathrm{U}_{\mathrm{R}} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{2}=\mathrm{U}_{3} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{2}
$$

For wet deposition, it is assumed that the rain scavenges $Q$ (the scavenging ratio) or about 200,000 times its volume of air. Using a particle concentration (volume fraction) $\mathrm{v}_{\mathrm{Q}}$ of $2 \times 10^{-11}$, this corresponds to the removal of $\mathrm{Qv}_{\mathrm{Q}}$ or $4 \times 10^{-6}$ volumes of aerosol per volume of rain. The total rate of particle removal by wet deposition is then $\mathrm{Qv}_{\mathrm{Q}} \mathrm{U}_{\mathrm{R}} \mathrm{A}_{\mathrm{W}} \mathrm{m}^{3} / \mathrm{h}$, thus the wet "transport velocity" $\mathrm{Qv}_{\mathrm{Q}} \mathrm{U}_{\mathrm{R}}$ is $4 \times 10^{-10} \mathrm{~m} / \mathrm{h}$.

For dry deposition, a typical deposition velocity $U_{Q}$ of $10 \mathrm{~m} / \mathrm{h}$ is selected yielding a rate of particle removal of $\mathrm{U}_{\mathrm{Q}} \mathrm{V}_{\mathrm{Q}} \mathrm{A}_{\mathrm{W}}$ or $2 \times 10^{-10} \mathrm{~A}_{\mathrm{W}} \mathrm{m}^{3} / \mathrm{h}$ corresponding to a transport velocity of $2 \times 10^{-10} \mathrm{~m} / \mathrm{h}$. Thus,

$$
\mathrm{U}_{4}=\mathrm{Qv}_{\mathrm{Q}} \mathrm{U}_{\mathrm{R}}+\mathrm{U}_{\mathrm{Q}} \mathrm{v}_{\mathrm{Q}}=\mathrm{v}_{\mathrm{Q}}\left(\mathrm{QU}_{\mathrm{R}}+\mathrm{U}_{\mathrm{Q}}\right)
$$

The total particle transport velocity $\mathrm{U}_{4}$ for wet and dry deposition is thus $6 \times 10^{-10} \mathrm{~m} / \mathrm{h}(67 \%$ wet and $33 \%$ dry) and the total D value $\mathrm{D}_{\mathrm{Qw}}$ is

$$
\mathrm{D}_{\mathrm{QW}}=\mathrm{U}_{4} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{7}
$$

where $Z_{7}$ is the aerosol $Z$ value.
The overall D value is given by

$$
\mathrm{D}_{12}=\mathrm{D}_{\mathrm{VW}}+\mathrm{D}_{\mathrm{RW}}+\mathrm{D}_{\mathrm{QW}}
$$

## 2. Water to Air ( $D_{21}$ )

Evaporation is treated as the reverse of absorption; thus $D_{21}$ is simply $D_{V w}$ as before.

## 3. Air to Soil ( $D_{13}$ )

A similar approach is adopted as for air-to-water transfer. Four processes are considered with rain dissolution $\left(\mathrm{D}_{\mathrm{RS}}\right)$ and wet and dry deposition $\left(\mathrm{D}_{\mathrm{QS}}\right)$ being treated identically except that the area term is now the air-soil area $\mathrm{A}_{\mathrm{S}}$.

For diffusion, the approach of Jury et al. (1983, 1984a,b,c) is used as described by Mackay and Stiver (1991) and Mackay (1991) in which three diffusive processes are treated. The air boundary layer is characterized by a mass transfer coefficient $\mathrm{k}_{\mathrm{S}}$ or $\mathrm{U}_{7}$ of $5 \mathrm{~m} / \mathrm{h}$, equal to that of the air-water mass transfer coefficient $\mathrm{k}_{\mathrm{A}}$ used in $\mathrm{D}_{12}$.

For diffusion in the soil air-pores, a molecular diffusivity of $0.02 \mathrm{~m}^{2} / \mathrm{h}$ is reduced to an effective diffusivity using a Millington-Quirk type of relationship by a factor of about 20 to $10^{-3} \mathrm{~m}^{2} / \mathrm{h}$. Combining this with a path length of 0.05 m gives an effective air-to-soil mass transfer coefficient $\mathrm{k}_{\mathrm{SA}}$ of $0.02 \mathrm{~m} / \mathrm{h}$, which is designated as $\mathrm{U}_{5}$.

Similarly, for diffusion in water a molecular diffusivity of $2 \times 10^{-6} \mathrm{~m}^{2} / \mathrm{h}$ is reduced by a factor of 20 to an effective diffusivity of $10^{-7} \mathrm{~m}^{2} / \mathrm{h}$, which is combined with a path length of 0.05 m to give an effective soil-to-water mass transfer coefficient of $\mathrm{k}_{\mathrm{SW}} 2 \times 10^{-6} \mathrm{~m} / \mathrm{h}$.

It is probable that capillary flow of water contributes to transport in the soil. For example, a rate of $7 \mathrm{~cm} /$ year would yield an equivalent water velocity of $8 \times 10^{-6} \mathrm{~m} / \mathrm{h}$, which exceeds the water diffusion rate by a factor of four. For illustrative purposes we thus select a water transport velocity or coefficient $U_{6}$ in the soil of $10 \times 10^{-6} \mathrm{~m} / \mathrm{h}$, recognizing that this will vary with rainfall characteristics and soil type. These soil processes are in parallel with boundary layer diffusion in series, so the final equations are

$$
\mathrm{D}_{\mathrm{VS}}=1 /\left[1 / \mathrm{D}_{\mathrm{s}}+1 /\left(\mathrm{D}_{\mathrm{SW}}+\mathrm{D}_{\mathrm{SA}}\right)\right]
$$

where

$$
\begin{aligned}
& \mathrm{D}_{\mathrm{S}}=\mathrm{U}_{7} \mathrm{~A}_{\mathrm{s}} \mathrm{Z}_{1} \quad\left(\mathrm{U}_{7}=5 \mathrm{~m} / \mathrm{h}\right) \\
& \mathrm{D}_{\mathrm{sw}}=\mathrm{U}_{6} \mathrm{~A}_{\mathrm{s}} \mathrm{Z}_{2} \quad\left(\mathrm{U}_{6}=10 \times 10^{-6} \mathrm{~m} / \mathrm{h}\right) \\
& \mathrm{D}_{\mathrm{SA}}=\mathrm{U}_{5} \mathrm{~A}_{\mathrm{S}} \mathrm{Z}_{1} \quad\left(\mathrm{U}_{5}=0.02 \mathrm{~m} / \mathrm{h}\right)
\end{aligned}
$$

where $A_{S}$ is the soil horizontal area.
Air-soil diffusion thus appears to be much slower than air-water diffusion because of the slow migration in the soil matrix. In practice, the result will be a nonuniform composition in the soil with the surface soil (which is much more accessible to the air than the deeper soil) being closer in fugacity to the atmosphere.

The overall D value is given as

$$
\mathrm{D}_{13}=\mathrm{D}_{\mathrm{vS}}+\mathrm{D}_{\mathrm{QS}}+\mathrm{D}_{\mathrm{RS}}
$$

## 4. Soil to Air ( $\mathrm{D}_{31}$ )

Evaporation is treated as the reverse of absorption, thus the D value is simply $\mathrm{D}_{\mathrm{vs}}$.

## 5. Water to Sediment ( $D_{24}$ )

Two processes are treated, diffusion and deposition.
Diffusion is characterized by a mass transfer coefficient $\mathrm{U}_{8}$ of $10^{-4} \mathrm{~m} / \mathrm{h}$, which can be regarded as a molecular diffusivity of $2 \times 10^{-6} \mathrm{~m}^{2} / \mathrm{h}$ divided by a path length of 0.02 m . In practice, bioturbation may contribute substantially to this exchange process, and in shallow water current-induced turbulence may also increase the rate of transport. Diffusion in association with organic colloids is not included. The D value is thus given as $\mathrm{U}_{8} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{2}$.

Deposition is assumed to occur at a rate of $5000 \mathrm{~m}^{3} / \mathrm{h}$, which corresponds to the addition of a depth of solids of $0.438 \mathrm{~cm} /$ year; thus $43.8 \%$ of the solids resident in the accessible bottom sediment is added each year. This rate is about $12 \mathrm{~cm}^{3} / \mathrm{m}^{2} \cdot$ day, which is high compared to values observed in large lakes. The velocity $\mathrm{U}_{9}$, corresponding to the addition of $5000 \mathrm{~m}^{3} / \mathrm{h}$ over the area of $10^{10} \mathrm{~m}^{2}$, is thus $5 \times 10^{-7} \mathrm{~m} / \mathrm{h}$.

It is assumed that of this $5000 \mathrm{~m}^{3} / \mathrm{h}$ deposited, $2000 \mathrm{~m}^{3} / \mathrm{h}$ or $40 \%$ is buried (yielding the advective flow rate in Table 1.5.1), $2000 \mathrm{~m}^{3} / \mathrm{h}$ or $40 \%$ is resuspended (as discussed later) and the remaining $20 \%$ is mineralized organic matter. The organic carbon balance is thus only approximate.

The transport velocities are thus:

$$
\begin{array}{ll}
\text { deposition } \mathrm{U}_{9} & 5.0 \times 10^{-7} \mathrm{~m} / \mathrm{h} \text { or } 0.438 \mathrm{~cm} / \mathrm{y} \\
\text { resuspension } \mathrm{U}_{10} & 2.0 \times 10^{-7} \mathrm{~m} / \mathrm{h} \text { or } 0.175 \mathrm{~cm} / \mathrm{y} \\
& \\
\text { burial } \mathrm{U}_{\mathrm{B}} & \begin{array}{l}
2.0 \times 10^{-7} \mathrm{~m} / \mathrm{h} \text { or } 0.175 \mathrm{~cm} / \mathrm{y} \\
\end{array} \quad \text { (included as an advective residence time of } 50,000 \mathrm{~h} \text { ) }
\end{array}
$$

The water-to-sediment D value is thus

$$
D_{24}=U_{8} A_{W} Z_{2}+U_{9} A_{W} Z_{5}
$$

where $\mathrm{Z}_{5}$ is the Z value of the particles in the water column.

## 6. Sediment to Water ( $\mathrm{D}_{42}$ )

This is treated similarly to $\mathrm{D}_{24}$ giving:

$$
\mathrm{D}_{42}=\mathrm{U}_{8} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{2}+\mathrm{U}_{10} \mathrm{~A}_{\mathrm{W}} \mathrm{Z}_{4}
$$

where $U_{10}$ is the sediment resuspension velocity of $2.0 \times 10^{-7} \mathrm{~m} / \mathrm{h}$ and $\mathrm{Z}_{4}$ is the Z value of the sediment solids.

## 7. Sediment Advection or Burial ( $\mathrm{D}_{\mathrm{A} 4}$ )

This $D$ value is $U_{B} A_{w} Z_{4}$, where $U_{B}$, the sediment burial rate, is $2.0 \times 10^{-7} \mathrm{~m} / \mathrm{h}$. It can be viewed as $G_{B} Z_{B 4}$, where $G_{B}$ is the total burial rate specified as $\mathrm{V}_{S} / \mathrm{t}_{\mathrm{B}}$ where $\mathrm{t}_{\mathrm{B}}$ (residence time) is $50,000 \mathrm{~h}$, and $\mathrm{V}_{\mathrm{S}}$ (the sediment volume) is the product of sediment depth $(0.01 \mathrm{~cm})$ and area $\mathrm{A}_{\mathrm{W}} . \mathrm{Z}_{4}, \mathrm{Z}_{\mathrm{B} 4}$ are the Z values of the sediment solids and of the bulk sediment, respectively. Since there are $20 \%$ solids, $\mathrm{Z}_{\mathrm{B} 4}$ is about $0.2 \mathrm{Z}_{4}$. There is a slight difference between these approaches because in the advection approach (which is used here) there is burial of water as well as solids.

## 8. Soil to Water Run-Off ( $\mathrm{D}_{32}$ )

It is assumed that there is run-off of water at a rate of $50 \%$ of the rain rate, i.e., the D value is

$$
\mathrm{D}=0.5 \mathrm{U}_{3} \mathrm{~A}_{\mathrm{s}} \mathrm{Z}_{2}=\mathrm{U}_{11} \mathrm{~A}_{\mathrm{s}} \mathrm{Z}_{2}
$$

thus the transport velocity term $\mathrm{U}_{11}$ is $0.5 \mathrm{U}_{3}$ or $5 \times 10^{-5} \mathrm{~m} / \mathrm{h}$.
For solids run-off it is assumed that this run-off water contains 200 parts per million by volume of solids; thus the corresponding velocity term $\mathrm{U}_{12}$ is $200 \times 10^{-6} \mathrm{U}_{11}$, i.e., $10^{-8} \mathrm{~m} / \mathrm{h}$. This corresponds to the loss of soil at a rate of about 0.1 mm per year. If these solids were completely deposited in the aquatic environment (which is about $1 / 10$ th the soil area), they would accumulate at about 0.1 cm per year, which is about a factor of four less than the deposition rate to sediments. The implication is that most of this deposition is of naturally generated organic carbon and from sources such as bank erosion.

## Summary

The twelve intermedia transport parameters are listed in Table 1.5.7 and the equations are summarized in Table 1.5.8.

## Algebraic Solution

Four mass balance equations can be written, one for each medium, resulting in a total of four unknown fugacities, enabling simple algebraic solution as shown in Table 1.5.9. From the four fugacities, the concentration, amounts and rates of all transport and transformation processes can be deduced, yielding a complete mass balance.

The new information from the Level III calculations are the intermedia transport data, i.e., the extent to which chemical discharged into one medium tends to migrate into another. This migration pattern depends strongly on the proportions of the chemical discharged into each medium; indeed, the relative amounts in each medium are largely a reflection of the locations of discharge. It is difficult to interpret these mass balance diagrams because, for example, chemical depositing from air to water may have been discharged to air, or to soil from which it evaporated, or even to water from which it is cycling to and from air.

To simplify this interpretation, it is best to conduct three separate Level III calculations in which unit amounts ( $1000 \mathrm{~kg} / \mathrm{h}$ ) are introduced individually into air, soil and water. Direct discharges to sediment are unlikely and are not

## TABLE 1.5.7

## Intermedia transport parameters

| $\mathbf{U}$ |  | $\mathbf{m} / \mathbf{h}$ | m/year |
| :--- | :--- | :--- | :--- |
| 1 | Air side, air-water MTC $*, \mathrm{k}_{\mathrm{A}}$ | 5 | 43,800 |
| 2 | Water side, air-water MTC, $\mathrm{k}_{\mathrm{W}}$ | 0.05 | 438 |
| 3 | Rain rate, $\mathrm{U}_{\mathrm{R}}$ | $10^{-4}$ | 0.876 |
| 4 | Aerosol deposition | $6 \times 10^{-10}$ | $5.256 \times 10^{-6}$ |
| 5 | Soil-air phase diffusion MTC, $\mathrm{k}_{\mathrm{SA}}$ | 0.02 | 175.2 |
| 6 | Soil-water phase diffusion MTC, $\mathrm{k}_{\mathrm{SW}}$ | $10 \times 10^{-6}$ | 0.0876 |
| 7 | Soil-air boundary layer MTC, $\mathrm{k}_{\mathrm{S}}$ | 5 | 43,800 |
| 8 | Sediment-water MTC | $10^{-4}$ | 0.876 |
| 9 | Sediment deposition | $5.0 \times 10^{-7}$ | 0.00438 |
| 10 | Sediment resuspension | $2.0 \times 10^{-7}$ | 0.00175 |
| 11 | Soil-water run-off | $5.0 \times 10^{-5}$ | 0.438 |
| 12 | Soil-solids run-off | $10^{-8}$ | $8.76 \times 10^{-5}$ |

[^0]TABLE 1.5.8

## Intermedia transport $D$ value equations



## TABLE 1.5.9

Level III solutions to mass balance equations

## Compartment

## Mass balance equations

Air
Water
Soil
Sediment
where
$\mathrm{E}_{1}+\mathrm{f}_{2} \mathrm{D}_{21}+\mathrm{f}_{3} \mathrm{D}_{31}=\mathrm{f}_{1} \mathrm{D}_{\mathrm{T} 1}$
$\mathrm{E}_{2}+\mathrm{f}_{1} \mathrm{D}_{12}+\mathrm{f}_{3} \mathrm{D}_{32}+\mathrm{f}_{4} \mathrm{D}_{42}=\mathrm{f}_{2} \mathrm{D}_{\mathrm{T} 2}$
$\mathrm{E}_{3}+\mathrm{f}_{1} \mathrm{D}_{13}=\mathrm{f}_{3} \mathrm{D}_{\mathrm{T} 3}$
$\mathrm{E}_{4}+\mathrm{f}_{2} \mathrm{D}_{24}=\mathrm{f}_{4} \mathrm{D}_{\mathrm{T} 4}$
$\mathrm{E}_{\mathrm{i}}$ is discharge rate, $\mathrm{E}_{4}$ usually being zero.
$\mathrm{D}_{\mathrm{T} 1}=\mathrm{D}_{\mathrm{R} 1}+\mathrm{D}_{\mathrm{A} 1}+\mathrm{D}_{12}+\mathrm{D}_{13}$
$\mathrm{D}_{\mathrm{T} 2}=\mathrm{D}_{\mathrm{R} 2}+\mathrm{D}_{\mathrm{A} 2}+\mathrm{D}_{21}+\mathrm{D}_{23}+\mathrm{D}_{24},\left(\mathrm{D}_{23}=0\right)$
$\mathrm{D}_{\mathrm{T} 3}=\mathrm{D}_{\mathrm{R} 3}+\mathrm{D}_{\mathrm{A} 3}+\mathrm{D}_{31}+\mathrm{D}_{32},\left(\mathrm{D}_{\mathrm{A} 3}=0\right)$
$\mathrm{D}_{\mathrm{T} 4}=\mathrm{D}_{\mathrm{R} 4}+\mathrm{D}_{\mathrm{A} 4}+\mathrm{D}_{42}$
Solutions:

$$
\begin{aligned}
\mathrm{f}_{2} & =\left[\mathrm{E}_{2}+\mathrm{J}_{1} \mathrm{~J}_{4} / \mathrm{J}_{3}+\mathrm{E}_{3} \mathrm{D}_{32} / \mathrm{D}_{\mathrm{T} 3}+\mathrm{E}_{4} \mathrm{D}_{42} / \mathrm{D}_{\mathrm{T} 4}\right] /\left(\mathrm{D}_{\mathrm{T} 2}-\mathrm{J}_{2} \mathrm{~J}_{4} / \mathrm{J}_{3}-\mathrm{D}_{24} \cdot \mathrm{D}_{42} / \mathrm{D}_{\mathrm{T} 4}\right) \\
\mathrm{f}_{1} & =\left(\mathrm{J}_{1}+\mathrm{f}_{2} \mathrm{~J}_{2}\right) / \mathrm{J}_{3} \\
\mathrm{f}_{3} & =\left(\mathrm{E}_{3}+\mathrm{f}_{1} \mathrm{D}_{13}\right) / \mathrm{D}_{\mathrm{T} 3} \\
\mathrm{f}_{4} & =\left(\mathrm{E}_{4}+\mathrm{f}_{2} \mathrm{D}_{24}\right) / \mathrm{D}_{\mathrm{T} 4}
\end{aligned}
$$

where

$$
\begin{aligned}
& \mathrm{J}_{1}=\mathrm{E}_{1} / \mathrm{D}_{\mathrm{T} 1}+\mathrm{E}_{3} \mathrm{D}_{31} /\left(\mathrm{D}_{\mathrm{T} 3} \cdot \mathrm{D}_{\mathrm{T} 1}\right) \\
& \mathrm{J}_{2}=\mathrm{D}_{21} / \mathrm{D}_{\mathrm{T} 1} \\
& \mathrm{~J}_{3}=1-\mathrm{D}_{31} \cdot \mathrm{D}_{13} /\left(\mathrm{D}_{\mathrm{T} 1} \cdot \mathrm{D}_{\mathrm{T} 3}\right) \\
& \mathrm{J}_{4}=\mathrm{D}_{12}+\mathrm{D}_{32} \cdot \mathrm{D}_{13} / \mathrm{D}_{\mathrm{T} 3}
\end{aligned}
$$

considered here. These calculations show clearly the extent to which intermedia transport occurs. If, for example, the intermedia D values are small compared to the reaction and advection values, the discharged chemical will tend to remain in the discharge or "source" medium with only a small proportion migrating to other media. Conversely, if the intermedia D values are relatively large, the chemical becomes very susceptible to intermedia transport. This behavior is observed for persistent substances such as PCBs, which have very low rates of reaction.

A direct assessment of multimedia behavior is thus possible by examining the proportions of chemical found at steady state in the "source" medium and in other media. For example, when discharged to water, an appreciable fraction of the benzene is found in air, whereas for atrazine, only a negligible fraction of atrazine reaches air.

## Linear Additivity or Superposition of Results

Because these equations are entirely linear, the solutions can be scaled linearly. The concentrations resulting from a discharge of $2000 \mathrm{~kg} / \mathrm{h}$ are simply twice those of $1000 \mathrm{~kg} / \mathrm{h}$. Further, if discharge of $1000 \mathrm{~kg} / \mathrm{h}$ to air causes 500 kg in water and discharge of $1000 \mathrm{~kg} / \mathrm{h}$ to soil causes 100 kg in water, then if both discharges occur simultaneously, there will be 600 kg in water. If the discharge to soil is increased to $3000 \mathrm{~kg} / \mathrm{h}$, the total amount in the water will rise to $(500+300)$ or 800 kg . It is thus possible to deduce the amount in any medium arising from any combination of discharge rates by scaling and adding the responses from the unit inputs. This "linear additivity principle" is more fully discussed by Stiver and Mackay (1989).

The persistence or residence time of the chemical is independent of the emission rate, but it does depend on the "mode of entry, i.e., into which compartment the chemical is emitted."

In the diagrams presented later, these three-unit ( $1000 \mathrm{~kg} / \mathrm{h}$ ) responses are given. Also, an illustrative "three discharge" mass balance is given in which a total of $1000 \mathrm{~kg} / \mathrm{h}$ is discharged, but in proportions judged to be typical of chemical use and discharge to the environment. For example, benzene is believed to be mostly discharged to air with minor amounts to soil and water.

Also given in the tables are the rates of reaction, advection and intermedia transport for each case.
The reader can deduce the fate of any desired discharge pattern by appropriate scaling and addition. It is important to emphasize that because the values of transport velocity parameters are only illustrative, actual environmental conditions may be quite different; thus, simulation of conditions in a specific region requires determination of appropriate parameter values as well as the site-specific dimensions, reaction rate constants and the physical-chemical properties which prevail at the desired temperature.

In total, the aim is to convey an impression of the likely environmental behavior of the chemical in a readily assimilable form.

### 1.6 DATA SOURCES AND PRESENTATION

### 1.6.1 Data Sources

Most physical properties such as molecular weight (MW, g/mol), melting point (m.p., ${ }^{\circ} \mathrm{C}$ ), boiling point (b.p., ${ }^{\circ} \mathrm{C}$ ), and density have been obtained from commonly used handbooks such as the CRC Handbook of Chemistry and Physics (Weast 1972, 1982; Lide 2003), Lange's Handbook of Chemistry (Dean 1979, 1985, 1992), Dreisbach's Physical Properties of Chemical Compounds, Vol. I, II and III (1955, 1959, 1961), Organic Solvents, Physical Properties and Methods of Purification (Riddick et al. 1986), The Merck Index (Windholz 1983, Budavari 1989) and several handbooks and compilations of chemical property data for pesticides. Notable are the text by Hartley and Graham-Bryce (1980), the Agrochemicals Handbook (Hartley and Kidd 1987), the Pesticide Manual (Worthing and co-workers 1983, 1987, 1991, Tomlin 1994), the CRC Handbook of Pesticides (Milne 1995), the Agrochemicals Desk Reference (Montgomery 1993) and the SCS/ARS/CES Pesticide Properties Database by Wauchope and co-workers (Wauchope et al. 1992, AugustijnBeckers et al. 1994, Hornsby et al. 1996). Other physical-chemical properties such as aqueous solubility, vapor pressure, octanol-water partition coefficient, Henry's law constant, bioconcentration factor and sorption coefficient have been obtained from scientific journals or other environmental handbooks, notably Verschueren's Handbook of Environmental Data on Organic Chemicals $(1977,1983)$ and Howard and co-workers' Handbook of Environmental Fate and Exposure Data, Vol. I, II, III and IV (1989, 1990, 1991 and 1993). Other important sources of vapor pressure are the CRC Handbook of Chemistry and Physics (Weast 1972, 1982), Lange’s Handbook of Chemistry (Dean 1992), the Handbook of Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds (Zwolinski and Wilhoit 1971), the Vapor Pressure of Pure Substances (Boublik et al. 1973, 1984), the Handbook of the Thermodynamics of Organic Compounds (Stephenson and Malanowski 1987). For aqueous solubilities, valuable sources include the IUPAC Solubility Data Series (Barton 1984, Horvath and Getzen 1985, Shaw 1989a,b) and Horvath's Halogenated Hydrocarbons, Solubility-Miscibility with Water (Horvath 1982). Octanol-water partition coefficients are conveniently obtained from the compilation by Leo et al. (1971), Hansch and Leo (1979), Hansch et al. (1995), and Sangster (1989, 1993), or can be calculated from molecular structure by the methods of Hansch and Leo (1979) or Rekker (1977). Lyman et al. (1982) and Boethling and Mackay (2000) also outline methods of estimating solubility, $\mathrm{K}_{\mathrm{Ow}}$, vapor pressure, and the bioconcentration factor for organic chemicals. The recent Handbook of Environmental Degradation Rates by Howard et al. (1991) is a valuable source of rate constants and half-lives.

The most reliable sources of data are the original citations of valuable experimental data in the reviewed scientific literature. Particularly reliable are those papers which contain a critical review of data from a number of sources as well as independent experimental determinations. Calculated or correlated values are viewed as being less reliable. The aim
in this work has been to gather sufficient experimental data with a list of citations to interpret them and select a "best" or "most likely" value.

### 1.6.2 Data Presentation

## Chemical Properties.

The emphasis in this handbook is on experimentally determined values rather than estimated values. The latter are included when there is a lack of experimental data. Included in the experimental data are indirect measurements using GC or HPLC retention times.

The names, formula, melting and boiling point and density data are self-explanatory.
The molar volumes are in some cases at the stated temperature and in other cases at the normal boiling point. Certain calculated molecular volumes are also used; thus the reader is cautioned to ensure that when using a molar volume in any correlation, it is correctly selected. In the case of polynuclear aromatic hydrocarbons, the Le Bas molar volume is regarded as suspect because of the compact nature of the multi-ring compounds. It should thus be regarded as merely an indication of relative volume, not an absolute volume.

Heats of fusion, $\Delta \mathrm{H}_{\text {fus }}$, are generally expressed in $\mathrm{kcal} / \mathrm{mol}$ or $\mathrm{kJ} / \mathrm{mol}$ and entropies of fusion, $\Delta \mathrm{S}_{\text {fus }}$ in $\mathrm{cal} / \mathrm{mol} \cdot \mathrm{K}$ (e.u. or entropy unit) or $\mathrm{J} / \mathrm{mol} \cdot \mathrm{K}$. The fugacity ratio F, as discussed in Section 1.2 .8 , is used to calculate the supercooled liquid vapor pressure or solubility for correlation purposes. In the case of liquids such as benzene, it is 1.0 . For solids it is a fraction representing the ratio of solid-to-liquid solubility or vapor pressure.

A wide variety of solubilities (in units of $\mathrm{g} / \mathrm{m}^{3}$ or the equivalent $\mathrm{mg} / \mathrm{L}$ ) have been reported. Experimental data have the method of determination indicated. In other compilations of data the reported value has merely been quoted from another secondary source. In some cases the value has been calculated. The abbreviations are generally self-explanatory and usually include two entries, the method of equilibration followed by the method of determination. From these values a single value is selected for inclusion in the summary data table. Vapor pressures and octanol-water partition coefficients are selected similarly.

The reader is advised to consult the original reference when using these values of bioconcentration factors (BCF), bioaccumulation factors $(\mathrm{BAF}), \mathrm{K}_{\mathrm{OC}}$ and $\mathrm{K}_{\mathrm{OM}}$, to ensure that conditions are as close as possible to those of specific interest.

The "Environmental Fate Rate Constants" refer to specific degradation processes rather than media. As far as possible the original numerical quantities are given and thus there is a variety of time units with some expressions being rate constants and others half-lives. The conversion is that the rate constant k is $0.693 / \mathrm{t}_{1 / 2}$ where $\mathrm{t}_{1 / 2}$ is the half-life.

From these data a set of medium-specific degradation reaction half-lives is selected for use in Levels II and III calculations. Emphasis is placed on the fastest and the most plausible degradation process for each of the environmental compartments considered. Instead of assuming an equal half-life for both the water and soil compartment as suggested by Howard et al. (1991), a slower active class (in the reactivity table described earlier) was assigned for soil and sediment compared to that of the water compartment. This is in part because the major degradation processes are often photolysis (or photooxidation) and biodegradation. There is an element of judgment in this selection, and it is desirable to explore the implications of selecting other values.

The "Half-life in the Environment" data reflect observations of the rate of disappearance of the chemical from a medium, without necessarily identifying the cause of mechanism of loss. For example, loss from water may be a combination of evaporation, biodegradation and photolysis. Clearly these times are highly variable and depend on factors such as temperature, meteorology and the nature of the media. Again, the reader is urged to consult the original references.

### 1.7 ILLUSTRATIVE QSPR PLOTS AND FATE CALCULATIONS

Illustrative QSPR plots and their interpretation are given in this section, followed by examples of Levels I, II and III fate calculations. A relatively simple evaluation of benzene is given first followed by the more complex evaluation of pentachlorophenol.

### 1.7.1 QSPR Plots for Mononuclear Aromatic Hydrocarbons

The physical-chemical data for mononuclear aromatics are plotted in the appropriate QSPR plots on Figures 1.7.1 to 1.7.5 (which are also Figures 3.2 .1 to 3.2 .5 for the mononuclear aromatic hydrocarbons in Chapter 3). These plots show that the data are relatively "well-behaved," there being consistency among the reported values for this homologous series. In the case of benzene this QSPR plot is of little value because this is a well-studied chemical, but for other lessstudied chemicals the plots are invaluable as a means of checking the reasonableness of data. The plots can also be used,
with appropriate caution, to estimate data for untested chemicals. We do not develop linear regressions of these data since we suggest that the plots be used directly for data estimation purposes. This enables the user to assess into account the values of similarly structured compounds and it gives a direct impression of likely error. We discuss, below, the general nature of the relationships and in particular the slopes of the QSPR plots.

Figures 1.7.1 to 1.7.4 show the dependence of the physical-chemical properties on Le Bas molar volume. Figure 1.7.1 shows that the solubilities of the monoaromatics decrease steadily with increasing molar volume. The vapor pressure data in Figure 1.7.2 are similar, but $\log \mathrm{K}_{\mathrm{OW}}$ in Figure 1.7.3 increases with increasing molar volume also in a linear fashion.


FIGURE 1.7.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 1.7.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 1.7.3 Octanol-water partition coefficient versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 1.7.4 Henry's law constant versus Le Bas molar volume for mononuclear aromatic hydrocarbons.
The plot between Henry's law constant and molar volume (Figure 1.7.4) is more scattered. Figure 1.7 .5 shows the oftenreported inverse relationship between octanol-water partition coefficient and the supercooled liquid solubility.

The QSPR plots show that an increase in molar volume by $100 \mathrm{~cm}^{3} / \mathrm{mol}$ generally causes:
(i) A decrease in $\log$ solubility by 2.5 units, i.e., a factor of $10^{2.5}$ or 316 ;
(ii) A decrease in $\log$ vapor pressure by 2.2 units, i.e., a factor of $10^{2.2}$ of 159 ;
(iii) An increase in $\log$ Henry's law constant of 0.3 (i.e., $2.5-2.2$ ) or a factor or $10^{0.3}$ or 2.0 ;
(iv) An increase in $\log \mathrm{K}_{\text {ow }}$ by 2.0 units, i.e., a factor of 100 .

The plot of $\log \mathrm{K}_{\text {ow }}$ versus log solubility thus has a slope of approximately $2.0 / 2.5$ or 0.8 . This slope of less than 1.0 has been verified experimentally by Chiou et al. (1982) and Bowman and Sans (1983). Its theoretical basis has been discussed in detail by Miller et al. (1985).


FIGURE 1.7.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for mononuclear aromatic hydrocarbons.

Similar inferences can be made for other homologous series such as the chlorobenzenes and PCBs. In such cases the property change caused by substitution of one chlorine can be deduced as is illustrated later for chlorophenols.

The "Half-life in the Environment" and "Environmental Fate Rate Constants" are medium-specific degradation reaction half-lives selected for use in Level II and Level III calculations. As discussed earlier, emphasis was based on the fastest and the most plausible degradation process for each of the environmental compartments considered.

In summary, the physical-chemical and environmental fate data listed result in the tabulated selected values of solubility, vapor pressure, $\mathrm{K}_{\mathrm{OW}}$, dissociation constant where appropriate and reaction half-lives at the end of each chapter. These values are used in the evaluative environmental calculations.

### 1.7.2 Evaluative Calculations for Benzene

The illustrative evaluative environmental calculations described here are presented in the following format. Levels I, II and III diagrams are assigned to separate pages, and the physical-chemical properties are included in the Level I diagram. Two types of Level III diagrams are given; one depicts the transport processes and the other the distribution among compartments.

## Level I

The Level I calculation suggests that if $100,000 \mathrm{~kg}$ ( 100 tonnes) of benzene are introduced into the $100,000 \mathrm{~km}^{2}$ environment, $99 \%$ will partition into air at a concentration of $9.9 \times 10^{-7} \mathrm{~g} / \mathrm{m}^{3}$ or about $1 \mu \mathrm{~g} / \mathrm{m}^{3}$. The water will contain nearly $1 \%$ at a low concentration of $4 \mu \mathrm{~g} / \mathrm{m}^{3}$ or equivalently $4 \mathrm{ng} / \mathrm{L}$. Soils would contain $5 \times 10^{-6} \mu \mathrm{~g} / \mathrm{g}$ and sediments about $9.7 \times 10^{-6} \mu \mathrm{~g} / \mathrm{g}$. These values would normally be undetectable as a result of the very low tendency of benzene to sorb to organic matter in these media. The fugacity is calculated to be $3.14 \times 10^{-5} \mathrm{~Pa}$. The dimensionless soil-water and sediment-water partition coefficients or ratios of Z values are 2.6 and 5.3 as a result of a $\mathrm{K}_{\mathrm{OC}}$ of about 55 and a few percent organic carbon in these media. There is little evidence of bioconcentration with a very low fish concentration of $3.0 \times 10^{-5} \mu \mathrm{~g} / \mathrm{g}$. The pie chart in Figure 1.7 .6 clearly shows that air is the primary medium of accumulation.

## Level II

The Level II calculation includes the half-lives of 17 h in air, 170 h in water, 550 h in soil and 1700 h in sediment. No reaction is included for suspended sediment or fish. The input of $1000 \mathrm{~kg} / \mathrm{h}$ results in an overall fugacity of $6 \times 10^{-6}$ Pa , which is about $20 \%$ of the Level I value. The concentrations and amounts in each medium are thus about $20 \%$ of the Level I values. The relative mass distribution is identical to Level I. The primary loss mechanism is reaction in air, which accounts for $802 \mathrm{~kg} / \mathrm{h}$ or $80.2 \%$ of the input. Most of the remainder is lost by advective outflow. The water, soil and sediment loss processes are unimportant largely because so little of the benzene is present in these media, but also

Chemical name: Benzene
Fugacity Level I calculations: (six-compartment model)


Fugacity, $f=3.142 \mathrm{E}-05$

| Compartment | Z | Concentration |  |  | Amount$\qquad$ kg | Amount\% |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{mol} / \mathrm{m}^{3} \cdot \mathrm{~Pa}$ | $\mathrm{mol} / \mathrm{m}^{3}$ | $\mathrm{g} / \mathrm{m}^{3}$ | $\mu \mathrm{g} / \mathrm{g}$ |  |  |
| Air (1) | $4.034 \mathrm{E}-04$ | $1.268 \mathrm{E}-08$ | 9.901E-07 | 8.251E-04 | $9.901 \mathrm{E}+04$ | $9.901 \mathrm{E}+01$ |
| Water (2) | 1.794E-03 | 5.638E-08 | 4.404E-06 | 4.404E-06 | 8.808E+02 | 8.808E-01 |
| Soil (3) | $4.764 \mathrm{E}-03$ | 1.497E-07 | 1.169E-05 | 4.871E-06 | 1.052E+02 | 1.052E-01 |
| Bottom sediment (4) | 9.527E-03 | $2.994 \mathrm{E}-07$ | $2.338 \mathrm{E}-05$ | 9.743E-06 | $2.338 \mathrm{E}+00$ | $2.338 \mathrm{E}-03$ |
| Suspended sediment (5) | 2.977E-02 | $9.355 \mathrm{E}-07$ | 7.307E-05 | 4.871E-05 | 7.307E-02 | 7.307E-05 |
| Biota (6) | 1.210E-02 | 3.803E-07 | 2.970E-05 | 2.970E-05 | 5.941E-03 | 5.941E-06 |
| Total |  |  |  |  | 1.000 E | $1.000 \mathrm{E}+02$ |

FIGURE 1.7.6 Level I fugacity calculations for benzene in a generic environment.
because of the slower reaction and advection rates. The overall residence time is 19.9 h ; thus, there is an inventory of benzene in the system of $19.9 \times 1000$ or 19900 kg . The pie chart in Figure 1.7.7 illustrates the dominance of air reaction and advection.

If the primary loss mechanism of atmospheric reaction is accepted as having a 17 h half-life, the D value is $1.6 \times 10^{9} \mathrm{~mol} / \mathrm{Pa} \cdot \mathrm{h}$. For any other process to compete with this would require a value of at least $10^{8} \mathrm{~mol} / \mathrm{Pa} \cdot \mathrm{h}$. This is achieved by advection $\left(4 \times 10^{8}\right)$, but the other processes range in D value from 19 (advection in bottom sediment) to $1.5 \times 10^{6}$ (reaction in water) and are thus a factor of over 100 or less. The implication is that the water reaction rate constant would have to be increased 100 -fold to become significant. The soil rate constant would require an increase by $10^{4}$ and the sediment by $10^{6}$. These are inconceivably large numbers corresponding to very short half-lives, thus the actual values of the rate constants in these media are relatively unimportant in this context. They need not be known accurately. The most sensitive quantity is clearly the atmospheric reaction rate.

The amounts in the compartments can be calculated easily from the total amount and the percentages of mass distribution in Level I. For example, the amount in water is $0.881 \%$ of 19877 kg or 175 kg .

## Level III

The Level III calculation includes an estimation of intermedia transport. Examination of the magnitude of the intermedia D values given in the fate diagram (Figure 1.7.8) suggests that air-water and air-soil transport are most important with water-sediment and soil-water transport being negligible in potential transfer rate. The magnitude of these larger intermedia

Chemical name: Benzene
Fugacity Level II calculations: (six-compartment model)

Distribution of removal rates


| Compartment | Half-life h | D Value |  | $\begin{gathered} \text { Concentration } \\ \mathrm{mol} / \mathrm{m}^{3} \\ \hline \end{gathered}$ | Loss |  | Total Removal \% |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Reaction mol/Pa.h | Advection mol/Pa.h |  | Reaction kg/h | Advection kg/h |  |
| Air (1) | 17 | $1.645 \mathrm{E}+09$ | $4.034 \mathrm{E}+08$ | $2.520 \mathrm{E}-09$ | $8.023 \mathrm{E}+02$ | $1.968 \mathrm{E}+02$ | $9.991 \mathrm{E}+01$ |
| Water (2) | 170 | $1.463 \mathrm{E}+06$ | $3.589 \mathrm{E}+05$ | $1.121 \mathrm{E}-08$ | 7.137E-01 | $1.751 \mathrm{E}-01$ | 8.888E-02 |
| Soil (3) | 550 | $5.402 \mathrm{E}+04$ | - | $2.975 \mathrm{E}-08$ | $2.635 \mathrm{E}-02$ | - | $2.635 \mathrm{E}-03$ |
| Bottom sediment (4) | 1700 | $3.884 \mathrm{E}+02$ | $1.905 \mathrm{E}+01$ | $5.950 \mathrm{E}-08$ | 1.895E-04 | 9.296E-06 | $1.988 \mathrm{E}-05$ |
| Suspended sediment (5) | 170 | $1.214 \mathrm{E}+02$ | $2.977 \mathrm{E}+01$ | $1.859 \mathrm{E}-07$ | $5.921 \mathrm{E}-05$ | $1.452 \mathrm{E}-05$ | 7.373E-06 |
| Biota (6) | 170 | $9.867 \mathrm{E}+00$ | $2.421 \mathrm{E}+00$ | 7.559E-08 | $4.814 \mathrm{E}-06$ | 1.181E-06 | 5.995E-07 |

Fugacity, f 6.246E-06 Pa
Total amount, M $2.545 \mathrm{E}+05 \mathrm{~mol}$ Total amount $1.988 \mathrm{E}+04 \mathrm{~kg}$
Total reaction $D$ value , $D_{R} \quad 1.646 \mathrm{E}+09 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$
Total advection D value, $\mathrm{D}_{\mathrm{A}} \quad 4.038 \mathrm{E}+08 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$
Total D value, DT $2.050 \mathrm{E}+09 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$
Total loss by reaction $\quad 8.030 \mathrm{E}+02 \mathrm{~kg} / \mathrm{h}$
Total loss by advection $\quad 1.970 \mathrm{E}+02 \mathrm{~kg} / \mathrm{h}$
Total loss $1.000 \mathrm{E}+03 \mathrm{~kg} / \mathrm{h}$
Reaction residence time, $\mathrm{t}_{\mathrm{R}} \quad 2.475 \mathrm{E}+01 \mathrm{~h}$
Advection residence time, $\mathrm{t}_{\mathrm{A}} \quad 1.009 \mathrm{E}+02 \mathrm{~h}$
Overall residence time, $t_{0} \quad 1.988 \mathrm{E}+01 \mathrm{~h}$
FIGURE 1.7.7 Level II fugacity calculations for benzene in a generic environment.
transport D values (approximately $10^{6} \mathrm{~mol} / \mathrm{Pa} \cdot \mathrm{h}$ ) compared to the atmospheric reaction and advection values of $10^{8}$ to $10^{9}$ suggests that reaction and advection will be very fast relative to transport.

The bulk Z values are similar for air and water to the values for the "pure" phases in Levels I and II, but they are lower for soil and sediment because of the "dilution" of the solid phase with air or water.

Chemical name: Benzene
Fugacity Level III calculations: (four-compartment model)


Phase Properties and Rates:

|  |  |  | D Value |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |
| Compartment | Bulk Z | Half-life | Reaction | Advection |  |
| ( | mol . Pa | h | mol/Pa.h | mol/Pa.h |  |
| Air (1) | $4.034 \mathrm{E}-04$ | $1.700 \mathrm{E}+01$ | $1.645 \mathrm{E}+09$ | $4.034 \mathrm{E}+08$ |  |
| Water (2) | $1.795 \mathrm{E}-03$ | $1.700 \mathrm{E}+02$ | $1.463 \mathrm{E}+06$ | $3.589 \mathrm{E}+05$ |  |
| Soil (3) | $3.001 \mathrm{E}-03$ | $5.500 \mathrm{E}+02$ | $6.806 \mathrm{E}+04$ | - |  |
| Sediment (4) | $3.341 \mathrm{E}-03$ | $1.700 \mathrm{E}+03$ | $6.810 \mathrm{E}+02$ | $3.341 \mathrm{E}+01$ |  |

Residence time (h) (A)ir Only (W)ater Only (S)oil Only A+W+S | Residence time (h) | (A)ir Only (W)ater Only (S)oil Only | A $+\mathrm{W}+\mathrm{S}$ |  |  |
| :--- | :--- | :--- | :--- | :--- |
| Overall residence time | $1.977 \mathrm{E}+01$ | $1.407 \mathrm{E}+02$ | $8.675 \mathrm{E}+01$ | $6.274 \mathrm{E}+01$ | $\begin{array}{lllll}\text { Reaction residence time } & 2.462 \mathrm{E}+01 & 1.752 \mathrm{E}+02 & 1.058 \mathrm{E}+02 & 7.796 \mathrm{E}+01\end{array}$ Advection residence time $1.004 \mathrm{E}+02 \quad 7.142 \mathrm{E}+02 \quad 4.813 \mathrm{E}+02 \quad 3.212 \mathrm{E}+02$

Phase Properties, Compositions, and Transport and Transformation Rates:

| Emission Scenario | Emission (kg/h) |  |  | Fugacity (Pa) |  |  |  | Concentration ( $\mathrm{g} / \mathrm{m}^{3}$ ) |  |  |  | Amount (kg) |  |  | $\begin{gathered} \text { Total } \\ \text { Amount (kg) } \\ \hline \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{E}_{1}$ | $\mathrm{E}_{2}$ | $\mathrm{E}_{3}$ | $\mathrm{f}_{1}$ | $\mathrm{f}_{2}$ | $\mathrm{f}_{3}$ | $\mathrm{f}_{4}$ | $\mathrm{C}_{1}$ | $\mathrm{C}_{2}$ | $\mathrm{C}_{3}$ | $\mathrm{C}_{4}$ | $\mathrm{w}_{1} \quad \mathrm{w}_{2}$ | $\mathrm{w}_{3}$ | $\mathrm{w}_{4}$ |  |
| (A)ir Only | 1000 | 0 | 0 | $6.249 \mathrm{E}-06$ | $2.023 \mathrm{E}-06$ | 5.781E-06 | $1.556 \mathrm{E}-06$ | $1.969 \mathrm{E}-07$ | $2.836 \mathrm{E}-07$ | 1.355E-06 | $4.059 \mathrm{E}-07$ | $1.969 \mathrm{E}+045.673 \mathrm{E}+01$ | $2.439 \mathrm{E}+01$ | $2.030 \mathrm{E}-01$ | $1.977 \mathrm{E}+04$ |
| (W)ater Only | 0 | 1000 | 0 | $2.002 \mathrm{E}-06$ | $4.775 \mathrm{E}-03$ | $1.852 \mathrm{E}-06$ | $3.671 \mathrm{E}-03$ | 6.308E-08 | 6.693E-04 | $4.341 \mathrm{E}-07$ | 9.579E-04 | $6.308 \mathrm{E}+031.339 \mathrm{E}+05$ | $7.814 \mathrm{E}+00$ | 4.790E+02 | $1.407 \mathrm{E}+05$ |
| (S)oil Only | 0 | 0 | 1000 | $5.676 \mathrm{E}-06$ | $4.999 \mathrm{E}-05$ | $1.599 \mathrm{E}-02$ | $3.843 \mathrm{E}-05$ | $1.788 \mathrm{E}-07$ | $7.007 \mathrm{E}-06$ | $3.748 \mathrm{E}-03$ | $1.003 \mathrm{E}-05$ | $1.788 \mathrm{E}+041.401 \mathrm{E}+03$ | 6.746E+04 | $5.015 \mathrm{E}+00$ | $8.675 \mathrm{E}+04$ |
| A+W+S | 600 | 300 | 00 | $4.918 \mathrm{E}-06$ | 39E-03 | 1.603E-03 | 106E-03 | $1.550 \mathrm{E}-07$ | $2.017 \mathrm{E}-04$ | 3.757E-04 | $2.886 \mathrm{E}-04$ | .550E+04 4.033E+04 | .763E+03 | 443E+02 | . 274 |


| Emission | Emission (kg/h) |  |  | Loss by Reaction (kg/h) |  |  |  | Loss by Advection (kg/h) |  |  | Intermedia Rate of Transport (kg/h) |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Scenario | $\mathrm{E}_{1}$ | $\mathrm{E}_{2}$ | $\mathrm{E}_{3}$ | $\mathrm{R}_{1}$ | $\mathrm{R}_{2}$ | $\mathrm{R}_{3}$ | R4 | $\mathrm{A}_{1}$ | $\mathrm{A}_{2}$ | $\mathrm{A}_{4}$ | $\mathrm{T}_{12}$ | $\mathrm{T}_{21}$ | $\mathrm{T}_{13}$ | $\mathrm{T}_{31}$ | $\mathrm{T}_{32}$ | $\mathrm{T}_{24}$ | $\mathrm{T}_{42}$ |
| (A)ir Only | 1000 | 0 | 0 | $8.028 \mathrm{E}+02$ | $2.312 \mathrm{E}-01$ | 3.073E-02 | 8.274E-05 | $1.969 \mathrm{E}+02$ | 5.673E-02 | 4.059E-06 | $4.202 \mathrm{E}-01$ | $1.358 \mathrm{E}-01$ | $3.617 \mathrm{E}-01$ | 3.273E-01 | 3.648E-03 | 3.071E-04 | $2.203 \mathrm{E}-04$ |
| (W)ater Only | 0 | 1000 | 0 | $2.572 \mathrm{E}+02$ | 5.457E+02 | $9.845 \mathrm{E}-03$ | 1.952E-01 | $6.308 \mathrm{E}+01$ | $1.339 \mathrm{E}+02$ | 9.579E-03 | $1.346 \mathrm{E}-01$ | $3.204 \mathrm{E}+02$ | $1.159 \mathrm{E}-01$ | 1.049E-01 | 1.169E-03 | 7.248E-01 | 5.200E-01 |
| (S)oil Only | 0 | 0 | 1000 | 7.290E+02 | $5.713 \mathrm{E}+00$ | $8.499 \mathrm{E}+01$ | $2.044 \mathrm{E}-03$ | $1.788 \mathrm{E}+02$ | $1.401 \mathrm{E}+00$ | 1.003E-04 | $3.816 \mathrm{E}-01$ | $3.354 \mathrm{E}+00$ | $3.285 \mathrm{E}-01$ | $9.052 \mathrm{E}+02$ | $1.009 \mathrm{E}+01$ | $7.588 \mathrm{E}-03$ | $5.444 \mathrm{E}-03$ |
| A $+\mathrm{W}+\mathrm{S}$ | 600 | 300 | 100 | 6.317E+02 | $1.644 \mathrm{E}+02$ | $8.521 \mathrm{E}+00$ | 5.883E-02 | $1.550 \mathrm{E}+02$ | 4.033E+01 | $2.886 \mathrm{E}-03$ | $3.306 \mathrm{E}-01$ | $9.653 \mathrm{E}+01$ | $2.846 \mathrm{E}-01$ | $9.075 \mathrm{E}+01$ | $1.011 \mathrm{E}+00$ | $2.184 \mathrm{E}-01$ | 1.567E-01 |

FIGURE 1.7.8 Level III fugacity calculations for benzene in a generic environment.

The first row describes the condition if $1000 \mathrm{~kg} / \mathrm{h}$ is emitted into the air. The result is similar to the Level II calculation with 19700 kg in air, 57 kg in water, 24 kg in soil and only 0.2 kg in sediment. It can be concluded that benzene discharged to the atmosphere has very little potential to enter other media. The rates of transfer from air to water and air to soil are both only about $0.4 \mathrm{~kg} / \mathrm{h}$. Even if the transfer coefficients were increased by a factor of 10 , the rates would remain negligible. The reason for this is the value of the mass transfer coefficients which control this transport process. The overall residence time is 19.8 hours, similar to Level II.

If $1000 \mathrm{~kg} / \mathrm{h}$ of benzene is discharged to water, as in the second row, there is predictably a much higher concentration in water (by a factor of over 2000). There is reaction of $546 \mathrm{~kg} / \mathrm{h}$ in water, advective outflow of $134 \mathrm{~kg} / \mathrm{h}$ and transfer to air of $320 \mathrm{~kg} / \mathrm{h}$ with negligible loss to sediment. The amount in the water is 134000 kg ; thus the residence time in the water is 134 h and the overall environmental residence time is a longer 140 hours. The key processes are thus reaction in water (half-life 170 h ), evaporation (half-life 290 h ) and advective outflow (residence time 1000 h ). The evaporation half-life can be calculated as $(0.693 \times$ mass in water)/rate of transfer, i.e., $(0.693 \times 133863) / 320=290 \mathrm{~h}$. Clearly, competition between reaction and evaporation in the water determines the overall fate. Ninety-five percent of the benzene discharged is now found in the water, and the concentration is a fairly high $6.7 \times 10^{-4} \mathrm{~g} / \mathrm{m}^{3}$, or $670 \mathrm{ng} / \mathrm{L}$.

The third row shows the fate if discharge is to soil. The amount in soil is 67460 kg , reflecting an overall 87 h residence time. The rate of reaction in soil is only $85 \mathrm{~kg} / \mathrm{h}$ and there is no advection; thus, the primary loss mechanism is transfer to air $\left(\mathrm{T}_{31}\right)$ at a rate of $905 \mathrm{~kg} / \mathrm{h}$, with a relatively minor $10 \mathrm{~kg} / \mathrm{h}$ to water by run-off. The net result is that the air concentrations are similar to those for air discharge and the soil acts only as a reservoir. The soil concentration of $3.75 \times 10^{-3} \mathrm{~g} / \mathrm{m}^{3}$ or $2.5 \times 10^{-3} \mathrm{\mu g} / \mathrm{g}$ or $2.5 \mathrm{ng} / \mathrm{g}$ is controlled almost entirely by the rate at which the benzene can evaporate.

The net result is that benzene behaves entirely differently when discharged to the three media. If discharged to air it reacts rapidly and advects with a residence time of 20 h with little transport to soil or water. If discharged to water it reacts and evaporates to air with a residence time of 140 h . If discharged to soil it mostly evaporates to air with a residence time in soil of 53 h .

The final scenario is a combination of discharges, $600 \mathrm{~kg} / \mathrm{h}$ to air, $300 \mathrm{~kg} / \mathrm{h}$ to water, and $100 \mathrm{~kg} / \mathrm{h}$ to soil. The concentrations, amounts and transport and transformation rates are merely linearly combined versions of the three initial scenarios. For example, the rate of reaction in air is now $632 \mathrm{~kg} / \mathrm{h}$. This is 0.6 of the first (air emission) rate of $803 \mathrm{~kg} / \mathrm{h}$, i.e., $482 \mathrm{~kg} / \mathrm{h}$, plus 0.3 of the second (water emission) rate of $257 \mathrm{~kg} / \mathrm{h}$, i.e., $77 \mathrm{~kg} / \mathrm{h}$ and 0.1 of the third (soil emission) rate of $729 \mathrm{~kg} / \mathrm{h}$, i.e., 73 kg yielding a total of $(482+77+73)$ or $632 \mathrm{~kg} / \mathrm{h}$. It is also apparent that the amount in the air of 15500 kg causing a concentration of $0.155 \mu \mathrm{~g} / \mathrm{m}^{3}$ is attributable to emissions to air $\left(0.6 \times 0.197\right.$ or $\left.0.118 \mu \mathrm{~g} / \mathrm{m}^{3}\right)$, emissions to water $\left(0.3 \times 0.063\right.$ or $\left.0.019 \mu \mathrm{~g} / \mathrm{m}^{3}\right)$ and emissions to soil ( $0.1 \times 0.179$ or $0.018 \mu \mathrm{~g} / \mathrm{m}^{3}$ ). The concentration in water of $2.0 \times 10^{-4} \mathrm{~g} / \mathrm{m}^{3}$ or $202 \mu \mathrm{~g} / \mathrm{m}^{3}$ or $\mathrm{ng} / \mathrm{L}$ is largely attributable to the discharges to water, which alone cause $0.3 \times 669$ or $200 \mu \mathrm{~g} / \mathrm{m}^{3}$. Although more is emitted to air, it contributes less than $1 \mu \mathrm{~g} / \mathrm{m}^{3}$ to the water with soil emissions accounting for about $1 \mu \mathrm{~g} / \mathrm{m}^{3}$. Similarly, the prevailing soil concentration is controlled by the rate of discharge to the soil.

In this multimedia discharge scenario the overall residence time is 59 hours, which can be viewed as $60 \%$ of the air residence time of $19.7 \mathrm{~h}, 30 \%$ of the water residence time of 140 h and $10 \%$ of the overall soil residence time of 53 h . The overall amount in the environment of $59,000 \mathrm{~kg}$ is thus largely controlled by the discharges to water, which account for $(0.3 \times 133863)$ or $40,000 \mathrm{~kg}$.

Figure 1.7.9 shows the distributions of mass and removal process rates for these four scenarios. Clearly, when benzene is discharged into a specific medium, most of the chemical is found in that medium. Only in the case of discharges to soil is an appreciable fraction found in another compartment, namely air. This is because benzene evaporates fairly rapidly from soil without being susceptible to reaction or advection.

Finally, it is interesting to note that the fugacity in this final case (in units of mPa ) are for the four media $5.0 \times 10^{-3}$, $1.4,1.6$ and 1.1. The soil, sediment and water are fairly close to equilibrium, with the air notably "under-saturated" by a factor of about 200. This is the result of the rapid loss processes from air.

### 1.7.3 QSPR Plots for Chlorophenols and Alkylphenols

These QSPR (quantitative structure-property relationship) plots display the usual approximately linear relationships similar to those of the alkyl and chlorinated aromatic hydrocarbons.

Most acid dissociation constants $\mathrm{pK}_{\mathrm{a}}$ exceed environmental pH values, the exceptions being the highly chlorinated phenols. As a result, these substances tend to have higher apparent solubilities in water because of dissociation. The structure-property relationships apply to the un-ionized or protonated species; thus, experimental data should preferably be "corrected" to eliminate the effect of ionization, thus eliminating pH effects.
Chemical name: Benzene
Level III Distribution

Emission to Water Only
$E_{1}=0$
$E_{2}=1000 \quad \mathrm{~kg} / \mathrm{h}$
$E_{3}=0$
$E_{1}=0$
$E_{2}=0$
$E_{3}=1000 \quad \mathrm{~kg} / \mathrm{h}$

| $E_{1}=600$ | $\mathrm{~kg} / \mathrm{h}$ |
| :--- | :--- |
| $E_{2}=300$ | $\mathrm{~kg} / \mathrm{h}$ |
| $E_{3}=100$ | $\mathrm{~kg} / \mathrm{h}$ |

$$
t_{0}=1.41 \mathrm{E}+02 \mathrm{~h}
$$

$t_{0}=8.67 E+01 h$
$t_{0}=6.27 E+01 h$

Legend
Reaction Advection

FIGURE 1.7.9 Level III fugacity distributions of benzene for four emission scenarios.
Figure 1.7 .10 shows that the chlorophenol solubilities behave similarly to other chemical series with slopes of about $0.62 \log$ units per $20.9 \mathrm{~cm}^{3} / \mathrm{mol}$, which is the volume difference resulting from substitution by one chlorine. The result is a factor of $10^{0.62}$ or 4.2 drop in solubility per chlorine. The alkylphenols have a lower slope of about 0.5 per $\mathrm{CH}_{2}$ and usually have higher solubilities at the same molar volume. The two sets of data are, however, generally similar.

The vapor pressure data in Figure 1.7.11 show a slope of about $0.60 \log$ units per $20.9 \mathrm{~cm}^{3} / \mathrm{mol}$ (i.e., a factor or 4.0 ) per chlorine. There is a lower slope for the alkylphenols, and they usually have higher vapor pressures, especially for the larger molecules.

The $\mathrm{K}_{\mathrm{ow}}$ data in Figure 1.7.12 show that the chlorophenols and alkylphenols differ in properties, there being more uncertainty about the $\mathrm{K}_{\mathrm{OW}}$ of the longer-chain phenols. The chlorophenols tend to partition more into octanol at the same molar volume and are thus expected to be more bioaccumulative. The slope of the chlorophenol line is about 0.78 $\log$ units per chlorine or a factor of 6.0. The alkylphenol slope is lower and about $0.36 \log$ units per $\mathrm{CH}_{2}$, i.e., a factor of 2.3.

The Henry's law constant data calculated as the ratio of vapor pressure to solubility in Figure 1.7.13 are quite scattered. There is little systematic variation with molar volume. Most values of $\log \mathrm{H}$ lie between -0.1 to -0 , i.e., H lies between 0.8 and 0.08 , and the resulting air-water partition coefficient $\mathrm{K}_{\mathrm{AW}}$ or $\mathrm{H} / \mathrm{RT}$ thus lies between $3 \times 10^{-4}$ and $3 \times 10^{-5}$.

Figure 1.7.14, the plot of $\log \mathrm{K}_{\mathrm{Ow}}$ versus log solubility, shows a relatively high slope of 1.25 for the chlorophenols and a lower slope of 0.70 for the alkylphenols.

Addition of a chlorine causes a drop in chlorophenol solubility in water by about $0.62 \log$ units, and $\mathrm{K}_{\mathrm{OW}}$ increases by about 0.78 log units. For the alkylphenols, addition of a methylene causes about a $0.50 \log$ unit drop in solubility in water, and $\mathrm{K}_{\mathrm{OW}}$ increases by only about $0.36 \log$ units. The slope of the $\log \mathrm{K}_{\mathrm{OW}}$ versus solubility lines are thus about $0.78 / 0.62$ or 1.25 for the chlorophenols and $0.36 / 0.5$ or 0.72 for the alkylphenols. An implication is that since $\mathrm{K}_{\mathrm{Ow}}$ can


FIGURE 1.7.10 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alkylphenols and chlorophenols.


FIGURE 1.7.11 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alkylphenols and chlorophenols.
be viewed as a ratio of "solubility" in octanol and solubility in water, the solubility of the chlorophenols in octanol increases by $(0.78-0.62)$ or $0.16 \log$ unit per chlorine, while for the alkylphenols the corresponding change is $(0.36-0.50)$ or $-0.14 \log$ unit, or a decrease of a factor of 1.4. The reasons for this difference are not known. The chlorophenols thus appear to have an unusually strong tendency to partition into octanol. Whether or not this tendency applies to lipid phases in biota or to organic carbon is not certain, but such a tendency is obviously of considerable interest when interpreting the toxicity and fate of these chemicals.

These data show clearly that the structure-property relationships which apply to hydrophobic organic chemicals such as the chloro- and alkyl-aromatics also apply to the phenols, but the relationships are more scattered and less well defined. The absolute values of properties differ greatly. This scatter is probably attributable, in part, to insufficient experimental data or errors in experimental measurements, to dissociation and to the greater polar character of these chemicals. It is not recommended that correlations developed for non-polar organic chemicals be applied to the phenols. Separate treatment of each homologous series is required.


FIGURE 1.7.12 Octanol-water partition coefficient versus Le Bas molar volume for alkylphenols and chlorophenols.


FIGURE 1.7.13 Henry's law constant versus Le Bas molar volume for alkylphenols and chlorophenols.

### 1.7.4 Evaluative Calculations for Pentachlorophenol

For dissociating compounds the environmental pH is specified and the calculation of Z values has been modified to include ionic species as discussed in Section 1.2.4. Generally, if discharge is to a compartment such as water, most chemical will be found in that compartment, and will react there, but a quantity does migrate to other compartments and is lost from these media. Three pie charts corresponding to discharges of $1000 \mathrm{~kg} / \mathrm{h}$ to air, water and soil are included. The percentage emission in each medium in this case has been selected to be 5,25 and $70 \%$ discharged to air, water and soil, respectively. A fourth pie chart with discharges to all three compartments is also given. This latter chart is in principle the linear sum of the first three, but since the overall residence times differ, the diagram with the longer residence time, and greater resident mass, tends to dominate.

Figures 1.7.15 to 1.7.18 show the mass distributions obtained in Level I calculations and the removal distribution from Level II fugacity calculation of pentachlorophenol (PCP) at two different environmental pHs for the generic


FIGURE 1.7.14 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alkylphenols and chlorophenols.
environment. Figures 1.7.19 to 1.7.22 show the corresponding Level III fugacity calculations. Both mass and removal distributions are shown in these figures for the four scenarios of discharges to air, water, soil, and mixed compartments.

## Level I

The Level I calculations for environmental pHs of 5.1 and 7 suggest that if $100,000 \mathrm{~kg}$ ( 100 tonnes) of pentachlorophenol (PCP) are introduced into the $100,000 \mathrm{~km}^{2}$ environment, most PCP will tend to be associated with soil. This is especially the case at low pH when the protonated form dominates. Very little partitions into air and only about $1 \%$ partitions into water. Soil contains most of the PCP. Sediments contain about $2 \%$. There is evidence of bioconcentration with a rather high fish concentration. Note that only four media (air, water, soil and bottom sediment) are depicted in the pie chart; therefore, the sum of the percent distribution figures is slightly less than $100 \%$. The air-water partition coefficient is very low. As pH increases, dissociation increases and there is a tendency for partitioning to water to become more important. Essentially, the capacity of water for the chemical increases. Partitioning to air is always negligible.

## Level II

The Level II calculations at pH 5.1 include the reaction half-lives of 550 h in air, 550 h in water, 1700 h in soil and 5500 h in sediment. No reaction is included for suspended sediment or fish. The steady-state input of $1000 \mathrm{~kg} / \mathrm{h}$ results in an overall fugacity of $3.43 \times 10^{-8} \mathrm{~Pa}$, which is about 24 times the Level I value. The concentrations and amounts in each medium are thus about 24 times the Level I values. The relative mass distribution is identical to Level I. The primary loss mechanism is reaction in soil, which accounts for $936 \mathrm{~kg} / \mathrm{h}$, or $94 \%$ of the input. Most of the remainder is lost by reaction and advection in water. The air and sediment loss processes are unimportant largely because so little of the PCP is present in these media. The overall residence time is 2373 h ; thus, there is an inventory of PCP in the system of $2373 \times 1000$ or $2,373,000 \mathrm{~kg}$.

The primary loss mechanism of soil reaction has a D value of $1.03 \times 10^{11}$; thus, for any other process to compete with this would require a D value of at least $10^{10} \mathrm{~mol} / \mathrm{Pa} \cdot \mathrm{h}$. The next largest D values are $3.19 \times 10^{9}$ and $2.53 \times 10^{9}$ for reaction and advection in water, which are about a factor of 30 smaller. Only if the water advection or reaction rates are increased by about this factor will these processes become significant. As pH increases, reaction in, and advection from, water increase in importance.

## Level III

The Level III diagrams (Figures 1.7.19 to 1.7.22 for the two pHs ) are regarded as the most realistic depictions of chemical fate.

This calculation includes an estimation of intermedia transport. Examination of the magnitude of the intermedia D values given in the fate diagrams suggest that water-sediment and air-soil transport are most important, with soil-water, and air-water exchange being slower. This chemical tends to be fairly immobile in terms of intermedia transport.

Chemical name: Pentachlorophenol
Fugacity Level I calculations: (six-compartment model) at data pH of 5.1

Physical-chemical properties:
Molecular weight $(\mathrm{g} / \mathrm{mol})$
Melting point $\left({ }^{( } \mathrm{C}\right)$
Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right)$
Vapor pressure $(\mathrm{Pa})$
log Kow
Fugacity ratio, F
Dissociation const, pKa

| Partition coefficients: |  |
| ---: | :--- |
| 266.34 | Henry's law constant |
| 174 | Air/water |
| 14 | Organic carbon, $\mathrm{K}_{\mathrm{OC}}$ |
| $4.15 \mathrm{E}-03$ | Bioconcentration factor, BCF |
| 5.05 | Soil/water |
| $3.36 \mathrm{E}-02$ | Sediment/water |
| 4.74 | Suspended sediment/water |
|  | Aerosol/water |

$Z$ values in water:

| $7.90 \mathrm{E}-02$ | at data pH | 5.1 |
| :--- | :--- | ---: |
| $3.19 \mathrm{E}-05$ | neutral | 3.849 |
| $4.60 \mathrm{E}+04$ | ionic | 8.817 |
| $5.61 \mathrm{E}+03$ | total | 12.666 |
| $2.21 \mathrm{E}+03$ | at environ. pH | 5.1 |
| $4.42 \mathrm{E}+03$ | neutral | 3.849 |
| $1.38 \mathrm{E}+04$ | ionic | 8.817 |
| $4.86 \mathrm{E}+07$ | total | 12.666 |



FIGURE 1.7.15 Level I fugacity calculations for PCP at data determination pH of 5.1.

The bulk Z values are similar for air and water to the values for the "pure" phases in Level I and II, but they are lower for soil and sediment because of the "dilution" of the solid soil and sediment phases with air or water.

The complete discussion of PCP fate as deduced in these calculations is beyond our scope, but to assist the reader we describe the behavior at a pH of 5.1 in some detail below.

These tabulated data are given in numerical and pictorial form in Figures 1.7.19 to 1.7.22. The first row of figures at the foot of Figure 1.7.19 describes the condition if $1000 \mathrm{~kg} / \mathrm{h}$ is emitted to the air. The result is similar to the Level II calculation with 65780 kg in air, 21070 kg in water, 504700 kg in soil and only 40800 kg in sediment. It can be concluded that PCP discharged to the atmosphere has fairly high potential to enter other media. The rate of transfer from air to

Chemical name: Pentachlorophenol
Fugacity Level II calculations: (six-compartment model) at data pH of 5.1

Distribution of removal rates


| Compartment | Half-life h | D Value |  | Concentration $\mathrm{mol} / \mathrm{m}^{3}$ | Loss |  | Total <br> Removal \% |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Reaction mol/Pa.h | Advection mol/Pa.h |  | Reaction kg/h | Advection kg/h |  |
| Air (1) | 550 | 5.08E+07 | 4.03E+08 | 1.38E-11 | 4.64E-01 | $3.68 \mathrm{E}+00$ | 4.14E-01 |
| Water (2) | 550 | $3.19 \mathrm{E}+09$ | $2.53 \mathrm{E}+09$ | $4.34 \mathrm{E}-07$ | $2.91 \mathrm{E}+01$ | $2.31 \mathrm{E}+01$ | $5.22 \mathrm{E}+00$ |
| Soil (3) | 1700 | 1.03E+11 | - | $9.58 \mathrm{E}-04$ | $9.36 \mathrm{E}+02$ | - | $9.36 \mathrm{E}+01$ |
| Bottom sediment (4) | 5500 | 7.05E+08 | $1.12 \mathrm{E}+08$ | 1.92E-03 | $6.43 E+00$ | $1.02 \mathrm{E}+00$ | 7.45E-01 |
| Suspended sediment (5) | - | - | - | 5.99E-03 | - | - | - |
| Biota (6) | - | - | - | $2.43 \mathrm{E}-03$ | - | - | - |

Fugacity, f $\quad 3.43 \mathrm{E}-08 \mathrm{~Pa}$

| Fugacity, f | $3.43 \mathrm{E}-08 \mathrm{~Pa}$ |
| ---: | :--- |
| Total amount, M | $8.91 \mathrm{E}+06 \mathrm{~mol}$ |
| Total amount | $2.37 \mathrm{E}+06 \mathrm{~kg}$ |
| Total reaction D value, $\mathrm{D}_{\mathrm{R}}$ | $1.06 \mathrm{E}+11 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$ |
| Total advection D value, $\mathrm{D}_{\mathrm{A}}$ | $2.94 \mathrm{E}+09 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$ |
| Total D value, $\mathrm{D}_{\mathrm{T}}$ | $1.09 \mathrm{E}+11 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$ |
| Total loss by reaction | $9.72 \mathrm{E}+02 \mathrm{~kg} / \mathrm{h}$ |
| Total loss by advection | $2.78 \mathrm{E}+01 \mathrm{~kg} / \mathrm{h}$ |
| Total loss | $1.00 \mathrm{E}+03 \mathrm{~kg} / \mathrm{h}$ |
| Reaction residence time, $\mathrm{t}_{\mathrm{R}}$ | $2.44 \mathrm{E}+03 \mathrm{~h}$ |
| Advection residence time, $\mathrm{t}_{\mathrm{A}}$ | $8.53 \mathrm{E}+04 \mathrm{~h}$ |
| Overall residence time, $\mathrm{t}_{\mathrm{o}}$ | $2.37 \mathrm{E}+03 \mathrm{~h}$ |

FIGURE 1.7.16 Level II fugacity calculations for PCP at data determination pH of 5.1.
water $\left(T_{12}\right)$ is about $54 \mathrm{~kg} / \mathrm{h}$ and that from air to soil $\left(\mathrm{T}_{13}\right) 206 \mathrm{~kg} / \mathrm{h}$. The reason for this is the value of the mass transfer coefficients which control this transport process. The overall residence time is 632 h .

If $1000 \mathrm{~kg} / \mathrm{h}$ of PCP is discharged to water, as in the second row, there is, as expected, a much higher concentration in water. There is reaction of $494 \mathrm{~kg} / \mathrm{h}$ in water, advective outflow of $392 \mathrm{~kg} / \mathrm{h}$ and transfer to air $\left(\mathrm{T}_{21}\right)$ of $2.90 \mathrm{~kg} / \mathrm{h}$ with

Chemical name: Pentachlorophenol
Fugacity Level I calculations: (six-compartment model) at environmental pH of 7

Physical-chemical properties:
Molecular weight $(\mathrm{g} / \mathrm{mol})$
Melting point $\left({ }^{( } \mathrm{C}\right)$
Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right)$
Vapor pressure $(\mathrm{Pa})$
log Kow
Fugacity ratio, F
Dissociation const, pKa

| Partition coefficients: |  |
| ---: | :--- |
| 266.34 | Henry's law constant |
| 174 | Air/water |
| 14 | Organic carbon, K Oc |
| $4.15 \mathrm{E}-03$ | Bioconcentration factor, BCF |
| 5.05 | Soil/water |
| $3.36 \mathrm{E}-02$ | Sediment/water |
| 4.74 | Suspended sediment/water |
|  | Aerosol/water |



FIGURE 1.7.17 Level I fugacity calculations for PCP at environmental pH of 7 .
substantial loss of $128 \mathrm{~kg} / \mathrm{h}$ to sediment. The amount in the water is $392,200 \mathrm{~kg}$; thus, the residence time in the water is 392 h , and the overall environmental residence time is a longer 1153 h . The key processes are thus reaction in water (half-life 550 h ) and advective outflow (residence time 1000 h ). The evaporation half-life can be calculated as $(0.693 \times$ mass in water)/rate of transfer, i.e., $(0.693 \times 392,200) / 2.90=93700 \mathrm{~h}$. Clearly competition between advection and reaction in the water determines the overall fate. Thirty-four percent of the PCP discharged is now found in the water and the concentration is fairly high, namely $1.96 \times 10^{-3} \mathrm{~g} / \mathrm{m}^{3}$ or $1.96 \mu \mathrm{~g} / \mathrm{L}$.

The third row shows the fate if PCP is discharged to soil. The amount in soil is 245100 kg , with only 7.43 kg in air. The overall residence time is 2452 hours, which is largely controlled by the reaction rate in soil. The rate of reaction in soil is $999 \mathrm{~kg} / \mathrm{h}$ and there is no advection; thus, the other loss mechanism is transfer to air $\left(\mathrm{T}_{31}\right)$ at a rate of $0.11 \mathrm{~kg} / \mathrm{h}$, with a relatively minor $0.8 \mathrm{~kg} / \mathrm{h}$ to water by run-off. The soil concentration of $0.136 \mathrm{~g} / \mathrm{m}^{3}$ is controlled almost entirely by the rate at which the PCP reacts.

Chemical name: Pentachlorophenol
Fugacity Level II calculations: (six-compartment model) at environmental pH of 7



Distribution of removal rates


Reaction Advection

| Compartment | Half-life <br> h | D Value |  | Concentration $\mathrm{mol} / \mathrm{m}^{3}$ | Loss |  | Total <br> Removal \% |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Reaction mol/Pa.h | Advection mol/Pa.h |  | Reaction kg/h | Advection kg/h |  |
| Air (1) | 550 | $5.08 \mathrm{E}+07$ | $4.03 \mathrm{E}+08$ | $3.59 \mathrm{E}-12$ | $1.20 \mathrm{E}-01$ | $9.56 \mathrm{E}-01$ | $1.08 \mathrm{E}-01$ |
| Water (2) | 550 | $1.77 \mathrm{E}+11$ | $1.41 \mathrm{E}+11$ | 6.26E-06 | $4.20 \mathrm{E}+02$ | $3.34 \mathrm{E}+02$ | $7.54 \mathrm{E}+01$ |
| Soil (3) | 1700 | $1.03 \mathrm{E}+11$ | - | $2.49 \mathrm{E}-04$ | $2.34 \mathrm{E}+02$ | - | $2.43 \mathrm{E}+01$ |
| Bottom sediment (4) | 5500 | 7.05E+08 | $1.12 \mathrm{E}+08$ | 4.97E-04 | $1.67 \mathrm{E}+00$ | $2.65 \mathrm{E}-01$ | 1.93E-01 |
| Suspended sediment (5) | - | - | - | $1.55 \mathrm{E}-03$ | - | - | - |
| Biota (6) | - | - | - | 6.32E-04 | - | - | - |


| Fugacity, f | $8.89 \mathrm{E}-09 \mathrm{~Pa}$ |
| ---: | :--- |
| Total amount, M | $3.54 \mathrm{E}+06 \mathrm{~mol}$ |
| Total amount | $9.44 \mathrm{E}+05 \mathrm{~kg}$ |
| Total reaction D value, $\mathrm{D}_{\mathrm{R}}$ | $2.80 \mathrm{E}+11 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$ |
| Total advection D value, $\mathrm{D}_{\mathrm{A}}$ | $1.41 \mathrm{E}+11 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$ |
| Total D value, $\mathrm{D}_{\mathrm{T}}$ | $4.21 \mathrm{E}+11 \mathrm{~mol} / \mathrm{Pa} . \mathrm{h}$ |
| Total loss by reaction | $6.65 \mathrm{E}+02 \mathrm{~kg} / \mathrm{h}$ |
| Total loss by advection | $3.35 \mathrm{E}+02 \mathrm{~kg} / \mathrm{h}$ |
| Total loss | $1.00 \mathrm{E}+03 \mathrm{~kg} / \mathrm{h}$ |
| Reaction residence time, $\mathrm{t}_{\mathrm{R}}$ | $1.42 \mathrm{E}+03 \mathrm{~h}$ |
| Advection residence time, $\mathrm{t}_{\mathrm{A}}$ | $2.82 \mathrm{E}+03 \mathrm{~h}$ |
| Overall residence time, $\mathrm{t}_{\mathrm{o}}$ | $9.44 \mathrm{E}+02 \mathrm{~h}$ |

FIGURE 1.7.18 Level II fugacity calculations for PCP at environmental pH of 7 .
The net result is that PCP behaves entirely differently when discharged to the three media. If discharged to air, it advects rapidly and reacts with a residence time of 632 h or about 26.3 days, with substantial transport to soil or water. If discharged to water, it reacts and evaporates to air with a residence time of 1153 h or 48 days. If discharged to soil, it mostly reacts with an overall residence time of about 2452 h or 102 days.

Chemical name: Pentachloropheno
Fugacity Level III calculations: (four-compartment model) at data pH of 5.1

Phase Properties and Rates:

|  |  |  | D Value |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | Bulk Z |  |
|  | Half-life | Reaction | Advection |  |  |
| Compartment | $\mathrm{mol} / \mathrm{m}^{3} . \mathrm{Pa}$ | h | mol/Pa.h | mol/Pa.h |  |
| Air (1) | $4.038 \mathrm{E}-04$ | $5.500 \mathrm{E}+02$ | $5.09 \mathrm{E}+07$ | $4.04 \mathrm{E}+08$ |  |
| Water (2) | $1.361 \mathrm{E}+01$ | $5.500 \mathrm{E}+02$ | $3.43 \mathrm{E}+09$ | $2.72 \mathrm{E}+09$ |  |
| Soil (3) | $1.399 \mathrm{E}+04$ | $1.700 \mathrm{E}+03$ | $1.03 \mathrm{E}+11$ | - |  |
| Sediment (4) | $1.120 \mathrm{E}+04$ | $5.500 \mathrm{E}+03$ | $7.05 \mathrm{E}+08$ | $1.12 \mathrm{E}+08$ |  |

Residence time (h) (A)ir Only (W)ater Only (S)oil Only $\quad$ A $+\mathrm{W}+\mathrm{S}$ \begin{tabular}{lllll}
Residence time (h) \& (A)ir Only (W)ater Only (S)oil Only \& A $+\mathrm{W}+\mathrm{S}$ <br>
\hline Overall residence time \& $6.324 \mathrm{E}+02$ \& $1.153 \mathrm{E}+03$ \& $2.452 \mathrm{E}+03$ \& $2.036 \mathrm{E}+03$

 Reaction residence time $1.974 \mathrm{E}+031.952 \mathrm{E}+03 \quad 2.453 \mathrm{E}+03 \quad 2.358 \mathrm{E}+03$ 

Advection residence time $9.304 \mathrm{E}+02$ \& $2.817 \mathrm{E}+03$ \& $6.090 \mathrm{E}+06$ \& $1.491 \mathrm{E}+04$ <br>
\hline
\end{tabular}

Phase Properties, Compositions, and Transport and Transformation Rates:

| Emission | Emission (kg/h) |  |  | Fugacity (Pa) |  |  |  | Concentration ( $\mathrm{g} / \mathrm{m}^{3}$ ) |  |  |  | Amount (kg) |  |  |  | $\begin{gathered} \text { Total } \\ \text { Amount (kg) } \\ \hline \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Scenario | $\mathrm{E}_{1}$ | $\mathrm{E}_{2}$ | $\mathrm{E}_{3}$ | $\mathrm{f}_{1}$ | $\mathrm{f}_{2}$ | $\mathrm{f}_{3}$ | $\mathrm{f}_{4}$ | $\mathrm{C}_{1}$ | $\mathrm{C}_{2}$ | $\mathrm{C}_{3}$ | $\mathrm{C}_{4}$ | $\mathrm{w}_{1}$ | $\mathrm{w}_{2}$ | $\mathrm{w}_{3}$ | $\mathrm{w}_{4}$ |  |
| (A)ir Only | 1000 | 0 | 0 | $6.116 \mathrm{E}-06$ | $2.907 \mathrm{E}-08$ | $7.526 \mathrm{E}-09$ | $2.736 \mathrm{E}-08$ | $6.578 \mathrm{E}-07$ | 1.054E-04 | $2.804 \mathrm{E}-02$ | 8.160E-02 | $6.578 \mathrm{E}+04$ | $2.107 \mathrm{E}+04$ | $5.047 \mathrm{E}+05$ | $4.080 \mathrm{E}+04$ | 6.324E+05 |
| (W)ater Only | 0 | 1000 | 0 | $1.772 \mathrm{E}-08$ | $5.410 \mathrm{E}-07$ | $2.180 \mathrm{E}-11$ | 5.092E-07 | 1.905E-09 | 1.961E-03 | 8.122E-05 | $1.519 \mathrm{E}+00$ | $1.905 \mathrm{E}+02$ | $3.922 \mathrm{E}+05$ | $1.462 \mathrm{E}+03$ | $7.593 \mathrm{E}+05$ | 1.153E+06 |
| (S)oil Only | 0 | 0 | 1000 | $6.909 \mathrm{E}-10$ | $4.359 \mathrm{E}-10$ | $3.655 \mathrm{E}-08$ | $4.103 \mathrm{E}-10$ | 7.430E-11 | 1.580E-06 | $1.362 \mathrm{E}-01$ | $1.224 \mathrm{E}-03$ | $7.430 \mathrm{E}+00$ | $3.160 \mathrm{E}+02$ | $2.451 \mathrm{E}+06$ | $6.118 \mathrm{E}+02$ | $2.452 \mathrm{E}+06$ |
| A+W+S | 50 | 250 | 700 | 3.107E-07 | 1.370E-07 | $2.597 \mathrm{E}-08$ | $1.290 \mathrm{E}-07$ | 3.342E-08 | 4.966E-04 | $9.674 \mathrm{E}-02$ | $3.846 \mathrm{E}-01$ | $3.342 \mathrm{E}+03$ | $9.933 \mathrm{E}+04$ | $1.741 \mathrm{E}+06$ | $1.923 \mathrm{E}+05$ | $2.036 \mathrm{E}+06$ |


| Emission <br> Scenario | Emission (kg/h) |  |  | Loss by Reaction (kg/h) |  |  |  | Loss by Advection (kg/h) |  |  | Intermedia Rate of Transport (kg/h) |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{E}_{1}$ | $\mathrm{E}_{2}$ | $\mathrm{E}_{3}$ | $\mathrm{R}_{1}$ | $\mathrm{R}_{2}$ | $\mathrm{R}_{3}$ | $\mathrm{R}_{4}$ | $\mathrm{A}_{1}$ | $\mathrm{A}_{2}$ | $\mathrm{A}_{4}$ | $\mathrm{T}_{12}$ | $\mathrm{T}_{21}$ | $\mathrm{T}_{13}$ | $\mathrm{T}_{31}$ | $\mathrm{T}_{32}$ | $\mathrm{T}_{24}$ | $\mathrm{T}_{42}$ |
| (A)ir Only | 1000 | 0 | 0 | $8.288 \mathrm{E}+01$ | $2.655 \mathrm{E}+01$ | $2.06 \mathrm{E}+02$ | $5.141 \mathrm{E}+00$ | $6.578 \mathrm{E}+02$ | $2.107 \mathrm{E}+01$ | 8.160E-01 | $5.358 \mathrm{E}+01$ | $1.557 \mathrm{E}-01$ | $2.059 \mathrm{E}+02$ | 2.278E-02 | $1.647 \mathrm{E}-01$ | $6.864 \mathrm{E}+00$ | 9.076E-01 |
| (W)ater Only | 0 | 1000 | 0 | $2.401 \mathrm{E}-01$ | $4.942 \mathrm{E}+02$ | 5.96E-01 | 9.567E+01 | $1.905 \mathrm{E}+00$ | 3.922E+02 | $1.519 \mathrm{E}+01$ | 1.552E-01 | $2.897 \mathrm{E}+00$ | 5.965E-01 | 6.599E-05 | 4.770E-04 | $1.278 \mathrm{E}+02$ | $1.689 \mathrm{E}+01$ |
| (S)oil Only | 0 | 0 | 1000 | $9.362 \mathrm{E}-03$ | $3.982 \mathrm{E}-01$ | $9.99 \mathrm{E}+02$ | 7.709E-02 | 7.430E-02 | 3.160E-01 | $1.224 \mathrm{E}-02$ | 6.052E-03 | $2.334 \mathrm{E}-03$ | $2.326 \mathrm{E}-02$ | $1.106 \mathrm{E}-01$ | 7.999E-01 | $1.029 \mathrm{E}-01$ | $1.361 \mathrm{E}-02$ |
| A+W+S | 50 | 250 | 700 | $4.211 \mathrm{E}+00$ | $1.252 \mathrm{E}+02$ | 7.10E+02 | $2.423 \mathrm{E}+01$ | $3.342 \mathrm{E}+01$ | $9.933 \mathrm{E}+01$ | $3.846 \mathrm{E}+00$ | $2.722 \mathrm{E}+00$ | $7.337 \mathrm{E}-01$ | $1.046 \mathrm{E}+01$ | 7.861E-02 | 5.863E-01 | $3.235 \mathrm{E}+01$ | $4.277 \mathrm{E}+00$ |

FIGURE 1.7.19 Level III fugacity calculations for PCP at pH of 5.1.

Chemical name: Pentachloropheno
Level III Distribution at data pH of 5.1
Emission to Air Only
Emission rates:

$$
\begin{aligned}
& \mathrm{E}_{1}=1000 \quad \mathrm{~kg} / \mathrm{h} \\
& \mathrm{E}_{2}=0 \\
& \mathrm{E}_{3}=0
\end{aligned}
$$

Overall residence time:
$t_{0}=6.32 E+02 h$
Distribution of mass:


$$
\begin{aligned}
& E_{1}=0 \\
& E_{2}=1000 \quad \mathrm{~kg} / \mathrm{h} \\
& E_{3}=0
\end{aligned}
$$

Emission to Water Only
$E_{1}=0$
$E_{2}=1000 \quad \mathrm{~kg} / \mathrm{h}$
$\mathrm{E}_{3}=0$
$\mathrm{t}_{\mathrm{O}}=1.15 \mathrm{E}+03 \mathrm{~h}$

$$
\mathrm{t}_{\mathrm{O}}=1.15 \mathrm{E}+03 \mathrm{~h}
$$


Emission to Soil Only

| $E_{1}=0$ |
| :--- |
| $E_{2}=0$ |
| $E_{3}=1000 \quad \mathrm{~kg} / \mathrm{h}$ |
| $t_{0}=2.45 \mathrm{E}+03 \mathrm{~h}$ |



FIGURE 1.7.20 Level III fugacity distributions of PCP for four emission scenarios at pH of 5.1.

The final scenario is a combination of discharges, $50 \mathrm{~kg} / \mathrm{h}$ to air, $250 \mathrm{~kg} / \mathrm{h}$ to water, and $700 \mathrm{~kg} / \mathrm{h}$ to soil (which are different from the often assumed equal emissions). The concentrations, amounts and transport and transformation rates are merely linearly combined versions of the three initial scenarios. For example, the rate of reaction in air is now $4.21 \mathrm{~kg} / \mathrm{h}$. This is 0.05 of the first (air emission) rate of $82.9 \mathrm{~kg} / \mathrm{h}$, i.e., $4.14 \mathrm{~kg} / \mathrm{h}$, plus 0.25 of the second (water emission) rate of $0.24 \mathrm{~kg} / \mathrm{h}$, i.e., $0.06 \mathrm{~kg} / \mathrm{h}$ and 0.7 of the third (soil emission) rate of $0.0094 \mathrm{~kg} / \mathrm{h}$, i.e., $0.0066 \mathrm{~kg} / \mathrm{h}$ yielding a total of $(4.14+0.06+0.0066)$ or $4.21 \mathrm{~kg} / \mathrm{h}$. It is also apparent that the amount in the air of 3342 kg causing a concentration of $3.342 \times 10^{-8} \mathrm{~g} / \mathrm{m}^{3}$ or $33 \mathrm{ng} / \mathrm{m}^{3}$ is attributable to emissions to air $\left(0.05 \times 658\right.$ or $\left.33 \mathrm{ng} / \mathrm{m}^{3}\right)$, emissions to water $(0.25 \times 1.9$ or $0.5 \mathrm{ng} / \mathrm{m}^{3}$ ) and emissions to soil $\left(0.7 \times 0.0743\right.$ or $\left.0.052 \mu \mathrm{~g} / \mathrm{m}^{3}\right)$. The concentration in water of $4.97 \times 10^{-4} \mathrm{~g} / \mathrm{m}^{3}$, or $497 \mathrm{ng} / \mathrm{L}$, is largely attributable to the discharges to water, which alone cause $0.25 \times 1.96 \times 10^{-3} \mathrm{~g} / \mathrm{m}^{3}$ or $4.9 \times 10^{-4} \mathrm{~g} / \mathrm{m}^{3}$ or $490 \mu \mathrm{~g} / \mathrm{m}^{3}$, or $490 \mathrm{ng} / \mathrm{L}$. Although more is emitted to soil, it contributes only about $1.1 \mu \mathrm{~g} / \mathrm{m}^{3}$ to the water with air emissions accounting for about $5.27 \mu \mathrm{~g} / \mathrm{m}^{3}$. Similarly, the prevailing soil concentration is controlled by the rate of discharge to the soil.

In this multimedia discharge scenario the overall residence time is 2036 h , which can be viewed as the sum of $5 \%$ of the air emission residence time of $632 \mathrm{~h}, 25 \%$ of the water emission residence time of 1153 h and $70 \%$ of the soil emission residence time of 2452 h . The overall amount in the environment of $2.04 \times 10^{6} \mathrm{~kg}$ is thus largely controlled by the discharges to soil and water.

Finally, it is interesting to note that the fugacities in this final case (in units of $\mu \mathrm{Pa}$ ) are for the four media: 0.31 (air), 0.137 (water), 0.026 (soil) and 0.129 (sediment). The media are fairly close to equilibrium, i.e., within a factor of about 5 of the average value.

At pH 7 , Figure 1.7.21, the capacity of water for PCP increases; thus, the water compartment becomes more important as do intermedia transport processes involving water such as wet deposition in dissolved form and run-off

Chemical name: Pentachloropheno
Fugacity Level III calculations: (four-compartment model) at environmental pH of 7


Phase Properties and Rates

|  |  |  | D Value |  |
| :--- | :---: | :---: | :---: | :---: |
|  |  |  | Bulk Z | Half-life | Reaction | Advection |
| :---: |
| Compartment |

Residence time (h) $\quad$ (A)ir Only (W)ater Only (S)oil Only $\quad \mathrm{A}+\mathrm{W}+\mathrm{S}$ Overall residence time $\quad 2.074 \mathrm{E}+03 \quad 4.588 \mathrm{E}+02 \quad 2.393 \mathrm{E}+03 \quad 1.894 \mathrm{E}+03$ Reaction residence time $2.319 \mathrm{E}+03 \quad 8.218 \mathrm{E}+02 \quad 2.426 \mathrm{E}+03 \quad 2.164 \mathrm{E}+03$ | Advection residence time $1.961 \mathrm{E}+04$ | $1.039 \mathrm{E}+03$ | $1.805 \mathrm{E}+05$ | $1.515 \mathrm{E}+04$ |
| :--- | :--- | :--- | :--- | :--- |

Phase Properties, Compositions, and Transport and Transformation Rates:

| Emission Scenario | Emission (kg/h) |  |  | Fugacity (Pa) |  |  |  | Concentration ( $\mathrm{g} / \mathrm{m}^{3}$ ) |  |  |  | Amount (kg) |  |  |  | Total Amount (kg) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{E}_{1}$ | $\mathrm{E}_{2}$ | $\mathrm{E}_{3}$ | $\mathrm{f}_{1}$ | $\mathrm{f}_{2}$ | $\mathrm{f}_{3}$ | $\mathrm{f}_{4}$ | $\mathrm{C}_{1}$ | $\mathrm{C}_{2}$ | $\mathrm{C}_{3}$ | $\mathrm{C}_{4}$ | $\mathrm{w}_{1}$ | $\mathrm{w}_{2}$ | $\mathrm{w}_{3}$ | $\mathrm{w}_{4}$ |  |
| (A)ir Only | 1000 | 0 | 0 | 4.907E-07 | 1.408E-09 | $2.958 \mathrm{E}-08$ | $1.328 \mathrm{E}-09$ | 5.278E-08 | $2.645 \mathrm{E}-04$ | 1.118E-01 | $4.158 \mathrm{E}-03$ | $5.278 \mathrm{E}+03$ | $5.290 \mathrm{E}+04$ | $2.013 \mathrm{E}+06$ | $2.078 \mathrm{E}+03$ | $2.074 \mathrm{E}+06$ |
| (W)ater Only | 0 | 1000 | 0 | $3.097 \mathrm{E}-11$ | $1.175 \mathrm{E}-08$ | $1.867 \mathrm{E}-12$ | $1.108 \mathrm{E}-08$ | $3.331 \mathrm{E}-12$ | $2.207 \mathrm{E}-03$ | 7.060E-06 | $3.467 \mathrm{E}-02$ | $3.331 \mathrm{E}-01$ | $4.413 \mathrm{E}+05$ | $1.271 \mathrm{E}+02$ | $1.733 \mathrm{E}+04$ | $4.588 \mathrm{E}+05$ |
| (S)oil Only | 0 | 0 | 1000 | $6.453 \mathrm{E}-10$ | $3.510 \mathrm{E}-10$ | $3.497 \mathrm{E}-08$ | $3.309 \mathrm{E}-10$ | 6.940E-11 | 6.592E-05 | $1.322 \mathrm{E}-01$ | $1.036 \mathrm{E}-03$ | $6.940 \mathrm{E}+00$ | $1.318 \mathrm{E}+04$ | $2.380 \mathrm{E}+06$ | $5.178 \mathrm{E}+02$ | $2.393 \mathrm{E}+06$ |
| A+W+S | 50 | 250 | 700 | $2.500 \mathrm{E}-08$ | $3.253 \mathrm{E}-09$ | $2.596 \mathrm{E}-08$ | 3.067E-09 | $2.688 \mathrm{E}-09$ | 6.110E-04 | $9.814 \mathrm{E}-02$ | 9.600E-03 | $2.688 \mathrm{E}+02$ | $1.222 \mathrm{E}+05$ | $1.766 \mathrm{E}+06$ | $4.800 \mathrm{E}+03$ | $1.894 \mathrm{E}+06$ |


| Emission | Emission (kg/h) |  |  | Loss by Reaction (kg/h) |  |  |  | Loss by Advection (kg/h) |  |  | Intermedia Rate of Transport (kg/h) |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Scenario | $\mathrm{E}_{1}$ | $\mathrm{E}_{2}$ | $\mathrm{E}_{3}$ | $\mathrm{R}_{1}$ | $\mathrm{R}_{2}$ | $\mathrm{R}_{3}$ | $\mathrm{R}_{4}$ | $\mathrm{A}_{1}$ | $\mathrm{A}_{2}$ | $\mathrm{A}_{4}$ | $\mathrm{T}_{12}$ | $\mathrm{T}_{21}$ | $\mathrm{T}_{13}$ | $\mathrm{T}_{31}$ | $\mathrm{T}_{32}$ | $\mathrm{T}_{24}$ | $\mathrm{T}_{42}$ |
| (A)ir Only | 1000 | 0 | 0 | $6.650 \mathrm{E}+00$ | 6.665E-02 | $8.21 \mathrm{E}+02$ | $2.618 \mathrm{E}-01$ | $5.278 \mathrm{E}+01$ | $5.290 \mathrm{E}+01$ | 4.156E-02 | $9.470 \mathrm{E}+01$ | $7.565 \mathrm{E}-03$ | $8.470 \mathrm{E}+02$ | $1.112 \mathrm{E}+00$ | $2.517 \mathrm{E}+01$ | $5.920 \mathrm{E}-01$ | $2.886 \mathrm{E}-01$ |
| (W)ater Only | 0 | 1000 | 0 | 4.197E-04 | $5.561 \mathrm{E}+02$ | 5.18E-02 | $2.184 \mathrm{E}+00$ | $3.331 \mathrm{E}-03$ | $4.413 \mathrm{E}+02$ | $3.467 \mathrm{E}-01$ | 5.977E-03 | 6.312E-02 | $5.346 \mathrm{E}-02$ | 7.020E-05 | $1.589 \mathrm{E}-03$ | $4.939 \mathrm{E}+00$ | $2.408 \mathrm{E}+00$ |
| (S)oil Only | 0 | 0 | 1000 | 8.745E-03 | $1.661 \mathrm{E}+01$ | $9.70 \mathrm{E}+02$ | 6.525E-02 | 6.940E-02 | $1.318 \mathrm{E}+01$ | 1.036E-02 | $1.245 \mathrm{E}-01$ | 1.885E-03 | $1.114 \mathrm{E}+00$ | $1.315 \mathrm{E}+00$ | $2.975 \mathrm{E}+01$ | 1.475E-01 | 7.193E-02 |
| A+W+S | 50 | 250 | 700 | $3.387 \mathrm{E}-01$ | $1.540 \mathrm{E}+02$ | $7.20 \mathrm{E}+02$ | 6.048E-01 | $2.688 \mathrm{E}+00$ | $1.222 \mathrm{E}+02$ | 9.600E-02 | $4.823 \mathrm{E}+00$ | $1.748 \mathrm{E}-02$ | $4.314 \mathrm{E}+01$ | $9.758 \mathrm{E}-01$ | $2.208 \mathrm{E}+01$ | $1.368 \mathrm{E}+00$ | 6.667E-01 |

FIGURE 1.7.21 Level III fugacity calculations for PCP at pH of 7.
Level III Distribution at environmental pH of 7

Emission to Air Only
Emission rates:

$$
\begin{aligned}
& \mathrm{E}_{1}=1000 \quad \mathrm{~kg} / \mathrm{h} \\
& \mathrm{E}_{2}=0 \\
& \mathrm{E}_{3}=0
\end{aligned}
$$

Overall residence time
$\mathrm{t}_{\mathrm{O}}=2.07 \mathrm{E}+03 \mathrm{~h}$
Distribution of mass:

Emission to Soil Only

| $E_{1}$ | $=0$ |
| ---: | :--- |
| $E_{2}$ | $=0$ |
| $E_{3}$ | $=1000 \quad \mathrm{~kg} / \mathrm{h}$ |
| $t_{0}$ | $=2.39 \mathrm{E}+03 \mathrm{~h}$ |



Emission to Air, Water and Soil

| $\mathrm{E}_{1}=50$ | $\mathrm{~kg} / \mathrm{h}$ |
| :--- | :--- |
| $\mathrm{E}_{2}=250$ | $\mathrm{~kg} / \mathrm{h}$ |
| $\mathrm{E}_{3}=700$ | $\mathrm{~kg} / \mathrm{h}$ |
| $\mathrm{t}_{0}=1.89 E+03 \mathrm{~h}$ |  |



Advection

FIGURE 1.7.22 Level III fugacity distributions of PCP for four emission scenarios at pH of 7 .
from soil to water. The net effect is that if discharged to air, the amounts transferred to soil and water increase as does the overall residence time. If discharged to water, there is less water to sediment transfer because of the reduced apparent hydrophobicity, and the residence time decreases. If discharged to soil, there is little effect of the pH increase because the PCP tends to remain there.

Similar diagrams could be prepared for other phenolic compounds at a range of pH values. The results suggest that the same broad patterns of behavior apply as for PCP but the residence times are generally shorter because of reduced hydrophobicity and more rapid reactions. The lower chlorinated phenols are relatively short-lived and are not subject to appreciable intermedia transport, i.e., when discharged to a medium they tend to remain there until degraded or advected. The longest persistence occurs when the chemical is present in soils.

Such simulations suggest that because of their relatively high water solubility which in combination with low vapor pressure causes low air-water partition coefficients, the phenols tend to remain in water or in soil and show little tendency to evaporate. Their environmental fate tends to be dominated by reaction in soil and water, and for the more sorptive species, in sediments. Their half-lives are relatively short, because of their susceptibility to degradation.

It is believed that examining these three behavior profiles, and their combination in the fourth, illustrate and explain the environmental fate characteristics of this and other chemicals. Important intermedia transport processes and levels in various media that arise from discharges into other media become clear. It is believed that the broad characteristics of environmental fate as described in the generic environment are generally applicable to other environments, albeit with differences attributable to changes in volumes, temperature, flow rates and compartment compositions.

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## 2 Aliphatic and Cyclic Hydrocarbons

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### 2.1 LIST OF CHEMICALS AND DATA COMPILATIONS

### 2.1.1 Saturated Hydrocarbons

### 2.1.1.1 Alkanes

2.1.1.1.1 Isobutane (2-Methylpropane)


Common Name: Isobutane
Synonym: 2-methylpropane
Chemical Name: 2-methylpropane
CAS Registry No: 75-28-5
Molecular Formula: $\mathrm{C}_{4} \mathrm{H}_{10}$
Molecular Weight: 58.122
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -159.4 (Weast 1984; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
-11.73 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.5490 \quad$ (Weast 1984) $0.5571,0.5509 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 105.9 (calculated-density, Stephenson \& Malanowski 1987; Ruelle \& Kesselring 1997) 96.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 19.121, $21.297\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 4.540 (Dreisbach 1959; Riddick et al. 1986)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
48.9 (shake flask-GC at atmospheric pressure, McAuliffe 1963, 1966)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$101783^{*} \quad\left(-11.609^{\circ} \mathrm{C}\right.$, static method-manometer, measured range -85.5 to $-11.609^{\circ} \mathrm{C}$, Aston et al. 1940)
$101325^{*} \quad\left(-11.7^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -109.2 to $-11.7^{\circ} \mathrm{C}$, Stull 1947)
348100 (calculated from determined exptl. data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.74808-882.80 /\left(240.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -75 to $30^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

357000 (interpolated-Antoine eq., temp range -86.57 to $18.88^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91048-946.35 /\left(246.68+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -86.57 to $18.88^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 5084.4 /(\mathrm{T} / \mathrm{K})]+7.250$; temp range -115 to $-34^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 5416.2 /(\mathrm{T} / \mathrm{K})]+7.349085$; temp range -109.5 to $137.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$312486,313702^{*}\left(21.07,21.22^{\circ} \mathrm{C}\right.$, vapor-liquid equilibrium, measured range $4.580-71.17^{\circ} \mathrm{C}$, Steele et al. 1976) 356600 (extrapolated-Antoine eq., temp range -87 to $7^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90148-946.35 /\left(246.68+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -87 to $7^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 ) $\log (\mathrm{P} / \mathrm{kPa})=6.00272-947.54 /\left(248.87+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 351130 (interpolated-Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.03538-946.35 /(-26.47+\mathrm{T} / \mathrm{K})$; temp range $186-280 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.83572-1470.08 /(3.99+\mathrm{T} / \mathrm{K})$; temp range $121-187 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93028-907.164 /(-30.14+\mathrm{T} / \mathrm{K})$; temp range $263-306 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.26924-1102.296 /(-2.12+\mathrm{T} / \mathrm{K})$; temp range $301-366 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.95371-1648.648 /(77.939+\mathrm{T} / \mathrm{K})$; temp range $361-408 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=31.2541-1.9532 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.806 \cdot \log (\mathrm{~T} / \mathrm{K})+8.9246 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+5.7501 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $114-408 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
118640
120000 (calculated-P/C, Mackay \& Shiu 1981)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.76 (shake flask-GC, Leo et al. 1975)
2.76 (recommended, Sangster 1993)
2.76 (recommended, Hansch et al. 1995)
(converted from $1 / \mathrm{K}_{\mathrm{AW}}=\mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$ reported as exptl., Hine \& Mookerjee 1975)
100980, 22090 (calculated-group contribution, bond contribution, Hine \& Mookerjee 1975)
116700 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$ and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=1.42 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=1.31 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 297 K , measured range 297-499 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{OH}}=1.28 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Greiner 1967; quoted, Altshuller \& Bufalini 1971)
$\mathrm{k}_{\mathrm{OH}}=(2.52 \pm 0.05) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
$\mathrm{k}_{\mathrm{O} 3}=2.0 \times 10^{-23} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , temp range 298-323 K (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=(2.29 \pm 0.06) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=(2.34 \pm 0.33) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(24.6 \pm 0.4)^{\circ} \mathrm{C}($ Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}} *=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=9.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (recommended, Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3} *=(1.10 \pm 0.2) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $298-523 \mathrm{~K}$, atmospheric $\mathrm{t}_{1 / 2}=1750$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)
$\mathrm{k}_{\mathrm{OH}}=7.38 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=6.50 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=9.8 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and an estimated lifetime was 59 h (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=9.8 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ recommended $)=9.9 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)$ $=7.90 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995) $\mathrm{k}_{\mathrm{OH}}{ }^{*}=2.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}{ }^{*}=10.6 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:

Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $\mathrm{t}_{1 / 2}=1750 \mathrm{~h}$ due to reaction with $\mathrm{NO}_{3}$ radical during the night at room temp., and $\mathrm{t}_{1 / 2}=82 \mathrm{~h}$ for reaction with OH radical (Bagley et al. 1990);
atmospheric lifetime was estimated to be 59 h , based on a photooxidation rate constant $\mathrm{k}=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ in summer daylight with OH radical (Altshuller 1991).

TABLE 2.1.1.1.1.1
Reported vapor pressures of isobutane (2-methylpropane) at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |




FIGURE 2.1.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for isobutane.

### 2.1.1.1.2 2,2-Dimethylpropane (Neopentane)



Common Name: 2,2-Dimethylpropane
Synonym: neopentane, tetramethylmethane
Chemical Name: 2,2-dimethylpropane
CAS Registry No: 463-82-1
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{12}$
Molecular Weight: 72.149
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-16.4 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
9.503 (Dreisbach 1959; Stephenson \& Malanowski 1987)
9.48 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.5910,0.5852 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959 ; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$122.10\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Wang et al. 1992)
$117.6 \quad\left(20^{\circ} \mathrm{C}\right.$, Stephenson \& Malanowski 1987)
118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
21.778, $22.753 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
3.255 (Dreisbach 1959; Chickos et al. 1999)
3.146 (Riddick et al. 1986)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 12.69 (exptl., Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
33.2 (shake flask-GC at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
177930* (Antoine eq. regression, temp range -112 to $9.8^{\circ} \mathrm{C}$, Stull 1947)
171350 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.73812-950.84 /\left(237.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -60 to $55^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

171586* (derived from compiled data, temp range -13.729 to $29.914^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=7.2034-1020.7 /\left(230.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -52 to $17.6^{\circ} \mathrm{C}$ (Antoine eq., solid, Zwolinski \& Wilhoit 1971)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=6.60427-883.42 /\left(227.782+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -13.729 to $29.914^{\circ} \mathrm{C}$ (Antoine eq., liquid, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 5648.6 /(\mathrm{T} / \mathrm{K})]+7.263947$; temp range -102 to $152.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
169019* (24.56 ${ }^{\circ} \mathrm{C}$, ebulliometry, measured range -5.128 to $40^{\circ} \mathrm{C}$, Osborn \& Douslin 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=6.60427-883.42 /\left(227.78+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -14 to $29^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 171300 (selected, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.89316-938.234 /\left(235.249+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 171520, 171450 (interpolated-Antoine eq.-III and IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=6.3283-1020.7 /(-43.15+\mathrm{T} / \mathrm{K})$; temp range $223-256 \mathrm{~K}$ (Antoine eq-I., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=7.07825-1372.459 /(-8.39+\mathrm{T} / \mathrm{K})$; temp range $223-256 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.76532-900.545 /(-43.111+\mathrm{T} / \mathrm{K})$; temp range $268-313 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.83935-937.641 /(-38.071+\mathrm{T} / \mathrm{K})$; temp range $257-315 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.08953-1080.237 /(-17.896+\mathrm{T} / \mathrm{K})$; temp range $312-385 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.26795-2114.713 /(128.175+\mathrm{T} / \mathrm{K})$; temp range $382-433 \mathrm{~K}$ (Antoine eq-VI, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=26.6662-1.9307 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.0448 \cdot \log (\mathrm{~T} / \mathrm{K})+7.4104 \times 10^{-9} \cdot(\mathrm{~T} / \mathrm{K})+3.9463 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $257-434 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
221000
(calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
125640, 334380
(calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
373000
(calculated-P/C, Mackay \& Shiu 1981)
213250
(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.11
2.95, 3.41, 3.22
3.30, 3.08
3.11
2.98
3.11
(shake flask-GC, Leo et al. 1975; Leo et al. 1971; Hansch \& Leo 1979)
(calculated-fragment const., Rekker 1977)
(calculated-MO, calculated- $\pi$ const., Bodor et al. 1989)
(recommended, Sangster 1989, 1993)
(calculated- $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, * data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *($ exptl $)=6.50 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ calc $)=5.27 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range 298-493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=6.50 \times 10^{11} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ calc $)=5.37 \times 10^{11} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 298 K (Greiner 1970)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=5.50 \times 10^{-15} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=(1.04 \pm 0.17) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=9.30 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}}=9.0 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Winer et al. 1979)
$\mathrm{k}_{\mathrm{OH}} *=8.49 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)
$\mathrm{k}_{\mathrm{OH}} *=8.48 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

TABLE 2.1.1.1.2.1
Reported vapor pressures of 2,2-dimethylpropane (neopentane) at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{a} / \mathrm{T})$ |  |  |  |
| $\log \mathrm{P}=\mathrm{A}[1-\Phi /(\mathrm{T} / \mathrm{K})]$ | $(4)$ |  |  |

Stull 1947

| summary of literature data |  | selected values |  |  |  | ebulliometry |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  | solid |  |  | liquid | $-5.128$ | 57818 |
| -102.0 | 133.3 | -52.0 | 4000 | -13.729 | 39997 |  |  |
| -85.4 | 666.6 | -48.0 | 5333 | -7.047 | 53329 | -0.301 | 70121 |
| -76.7 | 1333 | -45.0 | 6666 | -1.570 | 66661 | 4.577 | 84666 |
| -67.2 | 2666 | -41.9 | 7999 | 3.112 | 79993 | 9.500 | 101325 |
| -56.1 | 5333 | -37.4 | 10666 | 7.224 | 93326 | 14.472 | 120793 |
| -49.0 | 7999 | -33.8 | 13332 | 7.991 | 95992 | 19.492 | 143246 |
| -39.1 | 13332 | -27.0 | 19998 | 8.742 | 98659 | 24.560 | 169019 |
| -23.7 | 26667 | -21.8 | 26664 | 9.112 | 101325 | 29.675 | 198488 |
| -7.10 | 53329 | -17.6 | 33331 | 10.199 | 103991 | $\begin{aligned} & 34.838 \\ & 40.048 \end{aligned}$ | $\begin{aligned} & 232017 \\ & 270022 \end{aligned}$ |
| 9.50 | 101325 |  |  | 10.906 | 106658 |  |  |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 9.478 | 14.251 | 119990 | $40.048$ | $270022$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -16.6 | Antoine eq. |  | 17.324133322 |  | $\begin{aligned} & \text { Cox eq. } \\ & \text { eq. } 5 \end{aligned} \quad \mathrm{P} / \mathrm{mmHg}$ |  |
|  |  |  |  | 22.829 | 159987 |  |  |  |
|  |  | A | 7.2034 | 29.914 | 199984 | $\Phi$ | 282.650 |
|  |  | B | 1020.7 | 25.0 | 171586 | a 0.802264 |  |
|  |  | C | 230.0 |  |  | b $\quad-6.70026 \times 10^{-4}$ |  |
|  |  | temp range - | to $-17.6^{\circ} \mathrm{C}$ |  |  | $\stackrel{c}{c}$ | $\begin{aligned} & 11.22918 \times 10^{-7} \\ & \text { ange } 268-314 \mathrm{~K} \end{aligned}$ |
|  |  | pres. range | $250 \mathrm{mmHg}$ | $\text { eq. } 2$ | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  |  |  | A | 6.60427 | for temp range $268-314 \mathrm{~K}$ |  |
|  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ}$ | $\left.\mathrm{l}^{-1}\right)=$ | B | 883.42 |  |  |  |  |
|  |  | at $25^{\circ} \mathrm{C}$ | 21.85 | C | 227.782 |  |  |  |
|  |  | at bp | 22.75 | $\begin{aligned} & \text { temp range }-14 \text { to } 30^{\circ} \mathrm{C} \\ & \text { pressure } 300-1800 \mathrm{mmHg} \end{aligned}$ |  |  |  |  |
|  |  |  |  |  |  |  |  |



FIGURE 2.1.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2,2-dimethylpropane.

### 2.1.1.1.3 n-Butane

Common Name: $n$-Butane
Synonym: 1-butane
Chemical Name: $n$-butane
CAS Registry No: 106-97-8
Molecular Formula: $\mathrm{C}_{4} \mathrm{H}_{10}$
Molecular Weight: 58.122
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -138.3 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
$-0.50 \quad$ (Dreisbach 1959; Stephenson \& Malanowski 1987; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.5788,0.5730 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
$0.5786,0.5729 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $100.45,101.45 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 96.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 21.066, 22.393 $\quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$4.393 \quad$ Parks \& Huffman 1931) 4.661 (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 34.56 (exptl., Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
65.6 (shake flask-UV, Morrison \& Billett 1952)
67.0 (shake flask-UV, Claussen \& Polglase 1952)
72.7 (shake flask-GC, Franks et al. 1966)
61.4 (shake flask-GC, McAuliffe 1963, 1966)
61.66 (shake flask-GC, Coates et al. 1985)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
288200 (extrapolated-Antoine eq. regression, temp range -101.5 to $-0.5^{\circ} \mathrm{C}$, Stull 1947)
243050 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83029-945.9 /\left(240.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -60 to $30^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

242647 (derived from compiled data, temp range -77.62 to $18.88^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80896-935.56 /\left(238.73+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -77.62 to $18.88^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
242840 (extrapolated-Antoine eq., temp range -77 to $19^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80896-935.86 /\left(238.73+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -77 to $19^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
243000 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.93266-935.773 /\left(238.789+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
242810 (interpolated-Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93386-935.86 /(-34.52+\mathrm{T} / \mathrm{K})$; temp range $195-292 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.3327-1409.73 /(\mathrm{T} / \mathrm{K})$; temp range $135-213 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.07512-1007.247 /(-25.272+\mathrm{T} / \mathrm{K})$; temp range $273-321 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.32267-1161.1 /(-3.107+\mathrm{T} / \mathrm{K})$; temp range $316-383 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.04942-1770.348 /(84.979+\mathrm{T} / \mathrm{K})$; temp range $375-425 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=27.0441-1.9049 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.1805 \cdot \log (\mathrm{~T} / \mathrm{K})-6.6845 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+4.219 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $135-425 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$592440 \quad\left(57.01^{\circ} \mathrm{C}\right.$, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
$94240 \quad$ (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
82080, 22100 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
95900 (calculated-P/C, Mackay \& Shiu 1975; Mackay 1981; Mackay \& Shiu 1981)
80210 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
92910 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
2.89 (shake flask-GC, Leo et al. 1975)
2.89 (concn. ratio, Cramer 1977)
2.46, 2.84, 2.96 (calculated-f const., Rekker 1977)
2.89, 2.76
(Hansch \& Leo 1979)
2.79
(calculated-hydrophobicity const., Iwase et al. 1985)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
1.53 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}=9.8 \times 10^{-24} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range 298-323 K (Schubert \& Pease 1956)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=3.1 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=3.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=1.66 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=1.54 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range 298-495 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{OH}}=1.8 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with atmospheric $\mathrm{t}_{1 / 2}=2.4$ to 24 h at 300 K (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=1.8 \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ in polluted atmosphere at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=3.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate at $0.11 \mathrm{~d}^{-1}$ for the reaction with OH radical and an average OH concn of $1.2 \times 10^{6}$ molecules $/ \mathrm{cm}^{3}$ (Zafonte \& Bonamassa 1977)
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=(2.57-4.22) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{OH}}($ calc $)=2.71 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at at atmospheric pressure and 300 K (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=2.58 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a, 1984c)
$\mathrm{k}_{\mathrm{O} 3}<10^{-23} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $<6 \times 10^{-7} \mathrm{~d}^{-1}, \mathrm{k}_{\mathrm{OH}}=2.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.2 \mathrm{~d}^{-1}$ and $\mathrm{k}_{\mathrm{NO} 3}=3.6 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.0007 \mathrm{~d}^{-1}$ (Atkinson \& Carter 1984; Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=2.54 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}} *=2.54 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=6.5 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (Atkinson 1990; Altshuller 1991).
$\mathrm{k}_{\mathrm{NO}_{3}} *=(0.45 \pm 0.06) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $298-523 \mathrm{~K}$, atmospheric $\mathrm{t}_{1 / 2}=4300$ h during the night at room temp. (discharge flow system, Bagley et al. 1990)
atmospheric lifetime was estimated to be 54 h , based on the photooxidation reaction rate constant with OH radical during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}=(\leq 2.0-6.6) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296-298 \mathrm{~K}$ (Atkinson 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=6.70 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ recommended $)=4.3 \times 10^{-17} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2$ K (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=2.44 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}{ }^{*}=4.59 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}} *=2.37 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $230-400 \mathrm{~K}$ (relative rate method, DeMore \& Bayes 1999)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: $t_{1 / 2}=6.5 \mathrm{~h}$ in ambient air based on reaction with OH radicals at 300 K (Doyle et al. 1975);
photolysis $\mathrm{t}_{1 / 2}=2.4$ to 24 h (Darnall et al. 1976);
atmospheric lifetimes $\tau(\mathrm{calc})=4 \times 10^{7} \mathrm{~h}$ for reaction with $\mathrm{O}_{3}, \tau=107 \mathrm{~h}$ with OH radical and $\tau=32150 \mathrm{~h}$ with $\mathrm{NO}_{3}$ radical based on reaction rate constants and environmental concentrations of $\mathrm{OH}, \mathrm{NO}_{3}$ radicals and $\mathrm{O}_{3}$ in the gas phase (Atkinson \& Carter 1984);
atmospheric lifetimes $\tau($ calc $)=222 \mathrm{~h}$ for the reaction with OH radical, $\tau=4 \times 10^{7} \mathrm{~h}$ with $\mathrm{O}_{3}$ and $\tau=32150$ $h$ with $\mathrm{NO}_{3}$ radical based on the rate constants and environmental concentrations of $\mathrm{OH}, \mathrm{NO}_{3}$ radicals and $\mathrm{O}_{3}$ in the gas phase (Atkinson 1985);
atmospheric $t_{1 / 2}=4300 \mathrm{~h}$ due to reaction with $\mathrm{NO}_{3}$ during the night at room temp., and $\mathrm{t}_{1 / 2}=77 \mathrm{~h}$ for reaction with OH radical (Bagley et al. 1990);
atmospheric lifetime $\tau \sim 54 \mathrm{~h}$ based on a photooxidation reaction rate constant of $2.54 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ with OH radicals during summer daylight hours (Altshuller 1991).

### 2.1.1.1.4 2-Methylbutane (Isopentane)



Common Name: 2-Methylbutane
Synonym: Isopentane
Chemical Name: 2-methylbutane
CAS Registry No: 78-78-4
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{12} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{2} \mathrm{CH}_{3}$
Molecular Weight: 72.149
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -159.77 Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 27.875 27.88 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6197,0.6146 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959) 0.6193, $0.6142 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $116.5,117.47 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 5.1505 (Dreisbach 1959, Riddick et al. 1986)
5.13 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 45.23, 43.35 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
47.8 (shake flask-GC, McAuliffe 1963,1966)
46.9* $\quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $20-60^{\circ} \mathrm{C}$, Pavlova et al. 1966)
72.4; 49.6, $55.2 \quad\left(0,25^{\circ} \mathrm{C}\right.$, shake flask-GC, calculated-group contribution, Polak \& Lu 1973)
48.0
(shake flask-GC, Price 1976)
48.0 (selected, Riddick et al. 1986)
48.5* (IUPAC recommended best value, temp range $0-60^{\circ} \mathrm{C}$, Shaw 1989)
52.11* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-323.2 K,

Ma̧czyński et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$82790 \quad\left(22.04^{\circ} \mathrm{C}\right.$, Schumann et al. 1942)
83720* $\quad\left(22.44^{\circ} \mathrm{C}\right.$, manometer, temp range $16.291-28.587^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87372-1075.816 /\left(233.259+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $16.291-28.587^{\circ} \mathrm{C}$ (Antoine eq. from exptl.
data, manometer, Willingham et al. 1945)
99550* (Antoine eq. regression, temp range -82.9 to $27.8^{\circ} \mathrm{C}$, Stull 1947)
91740 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.78967-1020.012 /\left(223.097+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -45 to $75^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
91646* (extrapolated-Antoine eq, temp range -67.03 to $49.14^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83315-1040.73 /\left(235.455 \mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -67.03 to $49.14^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 6470.8 /(\mathrm{T} / \mathrm{K})]+7.544680$; temp range: -82.9 to $180.3^{\circ} \mathrm{C}$, (Antoine eq., Weast $1972-73$ ) 91730, 92100 (interpolated, Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.04913-1081.748 /\left(239.817+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -56 to $22.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Schumann et al. 1942, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.9333-1029.602 /\left(234.294+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $16.29-28.59^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
91660 (interpolated-Antoine eq., temp range -87 to $7^{\circ} \mathrm{C}$, Dean 1985)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91048-946.35 /\left(246.68+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -87 to $7^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
$91700 \quad$ (quoted, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.92023-1022.88 /\left(233.460+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range not specified (Antoine eq., Riddick et al. 1986) 91640 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.95805-1040.73 /(-37.705+\mathrm{T} / \mathrm{K})$; temp range $216-323 \mathrm{~K}$ (Antoine eq-I., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.32287-1279.08 /(-4.481+\mathrm{T} / \mathrm{K})$; temp range $300-460 \mathrm{~K}$ (Antoine eq-II., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.39629-1325.048 /(1.244+\mathrm{T} / \mathrm{K})$; temp range $320-391 \mathrm{~K}$ (Antoine eq-III., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.22589-1212.803 /(-12.958+\mathrm{T} / \mathrm{K})$; temp range $385-416 \mathrm{~K}$ (Antoine eq-IV., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.09160-3167.07 /(233.708+\mathrm{T} / \mathrm{K})$; temp range $412-460 \mathrm{~K}$ (Antoine eq-V., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=29.2963-2.1762 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.883 \cdot \log (\mathrm{~T} / \mathrm{K})-4.6512 \times 10^{-11} .(\mathrm{T} / \mathrm{K})+3.8997 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $113-460 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
140000 (calculated-P/C, Mackay et al. 1979; Mackay 1981)
138000; 140000, 139000, 134700 (recommended; calculated-P/C, Mackay \& Shiu 1981))
138210 (selected, Mills et al. 1982)
138290 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.30 (calculated- $\pi$ constant, Hansch et al. 1968)
2.41 (calculated-MCI $\chi$, Murray et al. 1975)
2.83 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
2.4698 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, * data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=2.0 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with atmospheric $\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ (Lloyd 1976, Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(3.78 \pm 0.07) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=(3.97 \pm 0.11) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984 c )
$\mathrm{k}_{\mathrm{OH}}=3.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=3.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990, 1991; Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3} *=(1.60 \pm 0.2) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $298-523 \mathrm{~K}$, atmospheric $\mathrm{t}_{1 / 2}=1200 \mathrm{~h}$ during the night at room temp. (discharge flow system, Bagley et al. 1990)
$\mathrm{k}_{\mathrm{OH}}=3.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ at 298 K , estimated atmospheric lifetime of 36 h (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=1.56 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=2.49 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}=3.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}{ }^{*}=1.62 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $2.0 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976) with atmospheric $t_{1 / 2}=2.4-24 \mathrm{~h}$ (Darnall et al. 1976);
atmospheric $t_{1 / 2}=1200 \mathrm{~h}$ due to reaction with $\mathrm{NO}_{3}$ radical during the night at room temp., and $\mathrm{t}_{1 / 2}=50$ for reaction with OH radical (Bagley et al. 1990);
atmospheric lifetime of 36 h , based on rate constant of $3.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with OH radicals during summer daylight (Altshuller 1991).

## TABLE 2.1.1.1.4.1

Reported aqueous solubilities of 2-methylbutane (isopentane) at various temperatures

| Pavlova et al. 1966 |  | Polak \& Lu 1973 |  | Shaw 1989a |  | Ma̧czyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| in IUPAC 1989 |  | shake flask-GC/FID |  | IUPAC recommended |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 20 | 46.9 | 0 | 72.4 | 0 | 72 | 0 | 68.14 |
| 40 | 57.7 | 25 | 49.6 | 20 | 47 | 20 | 56.12 |
| 50 | 70.1 |  |  | 25 | 48.5 | 25 | 52.11 |
| 60 | 79.3 |  |  | 30 | 51 | 40 | 52.11 |
|  |  |  |  | 40 | 58 | 50 | 56.12 |
|  |  |  |  | 50 | 70 |  |  |
|  |  |  |  | 60 | 79 |  |  |



FIGURE 2.1.1.1.4.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 2-methylbutane.

TABLE 2.1.1.1.4.2
Reported vapor pressures of 2-methylbutane (isopentane) at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{align*}
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)  \tag{2}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})  \tag{3}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{~T} / \mathrm{K}) \\
& \ln \left(\mathrm{P} / \mathrm{P}_{\mathrm{ref}}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right) \tag{5}
\end{align*}
$$

Willingham et al. 1945
Stull 1947

| ebulliometry |  | summary of literature data |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 16.291 | 66760 | -82.9 | 133.3 | -57.03 | 1333 | 25.517 | 93326 |
| 22.435 | 83722 | -65.8 | 666.6 | -47.32 | 2666 | 26.320 | 95992 |
| 26.773 | 97608 | -57.0 | 1333 | -41.14 | 4000 | 27.156 | 98659 |
| 27.24 | 99207 | -47.3. | 2666 | -36.49 | 5333 | 27.875 | 101325 |
| 27.673 | 100700 | -36.5 | 5333 | -32.74 | 6666 | 25.0 | 91646 |
| 28.16 | 102402 | -29.6 | 7999 | -29.56 | 7999 |  |  |
| 28.587 | 103922 | -20.2 | 13332 | -24.35 | 10666 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | -5.90 | 26664 | -20.11 | 13332 | A | 6.83315 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 27.852 | 10.5 | 53329 | -11.97 | 19998 | B | 1040.73 |
|  |  | 27.8 | 101325 | -5.81 | 26664 | C | 235.445 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | -0.79 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | 28.875 |
| A | 6.78967 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -159.7 | 3.47 | 39997 | $\Delta \mathrm{H}_{\mathrm{v}} /$ |  |
| B | 1020.012 |  |  | 10.53 | 53329 | at $25^{\circ} \mathrm{C}$ | 24.84 |
| C | 233.097 |  |  | 16.293 | 66661 | at bp | 24.69 |
|  |  |  |  | 21.208 | 79993 |  |  |



FIGURE 2.1.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylbutane.

### 2.1.1.1.5 2,2-Dimethylbutane



Common Name: 2,2-Dimethylbutane
Synonym: neohexane, dimethylpropylmethane
Chemical Name: 2,2-dimethylbutane
CAS Registry No: 75-83-2
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{14} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right)_{2} \mathrm{CH}_{2} \mathrm{CH}_{3}$
Molecular Weight: 86.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-99.8 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
49.73 (Lide 2003)

Density (g/cm ${ }^{3}$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.6492,0.6445\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
132.74, 133.71
$\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$5.791 \quad$ (Dreisbach 1959; Riddick et al. 1986)
$5.4,0.28,0.58 \quad\left(-146.35,-132.35,-98.95^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
45.88, 42.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
18.4 (shake flask-GC, McAuliffe 1963,1966)
39.4, $23.8 \quad\left(0,25^{\circ} \mathrm{C}\right.$, shake flask-GC, Polak \& Lu 1973)
21.2 (shake flask-GC, Price 1976)
21.2 (shake flask-GC, Krzyzanowska, Szeliga 1978)
18.0 (selected Riddick et al. 1986)
21.0 (IUPAC recommended best value, Shaw 1989)
19.63 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$43320 \quad\left(24.47^{\circ} \mathrm{C}\right.$, manometer, temp range $15.376-50.529^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.75483-1081.176 /\left(229.343+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.376-50.529^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, manometer, Willingham et al. 1945)
43480 (Antoine eq. regression, temp range -69.3 to $49.7^{\circ} \mathrm{C}$, Stull 1947)
$42570 \quad\left(25^{\circ} \mathrm{C}\right.$, Nicolini \& Laffitte 1949)
42540 (calculated from determined data, Dreisbach 1959; quoted, Hine \& Mookerjee 1975) $\log (\mathrm{P} / \mathrm{mmHg})=6.75483-1081.176 /\left(229.343+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -25 to $95^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
42543 (interpolated-Antoine eq., temp range -41.5 to $72.8^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.75483-1081.176 /\left(229.343+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -41.5 to $72.8^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \&
Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7271.0 /(\mathrm{T} / \mathrm{K})]+7.84130$; temp range -69.3 to $49.7^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
42585, 42550 (interpolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.88698-1085.038 /\left(229.817+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.376-50.53^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.87001-1080.723 /\left(229.842+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-45^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Nicolini \& Laffitte 1949, Boublik et al. 1984)

42540 (interpolated-Antoine eq., temp range -42 to $73^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.75483-1081.176 /\left(229.34+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -42 to $73^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
42700 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.87963-1081.14 /\left(229.349+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 42560 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.87731-1079.789 /(-43.978+\mathrm{T} / \mathrm{K})$; temp range $293-324 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=33.1285-2.4527 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.2016 \cdot \log (\mathrm{~T} / \mathrm{K})-4.7077 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+4.1755 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $174-489 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 173000 | $($ calculated-P/C, Mackay \& Shiu 1981) |
| :--- | :--- |
| 196800 | (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975) |
| 196800,49430 | (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 173180 | (calculated-P/C, Eastcott et al. 1988) |
| 188040 | (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988) |
| 153890 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.82 (calculated-fragment const., Valvani et al. 1981)
3.25 (calculated- $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.82 (recommended, Sangster 1993)
3.82 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=(2.66 \pm 0.08) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984 c )
$\mathrm{k}_{\mathrm{OH}}=(2.59-6.16) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297-299 \mathrm{~K}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}} *=(2.22-0.36) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299 K , measured range $245-328 \mathrm{~K}$ (relative rate method, Harris \& Kerr 1988; Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=2.32 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}} *=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

### 2.1.1.1.6 <br> 2,3-Dimethylbutane



Common Name: 2,3-Dimethylbutane
Synonym: diisopropyl
Chemical Name: 2,3-dimethylbutane
CAS Registry No: 79-29-8
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{14} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{3}$
Molecular Weight: 86.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-128.10 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 57.93 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.6616,0.6570 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986) 0.6616 (Weast 1984)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $130.25,131.16 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
29.12, $27.275 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1959) 29.125, $27.276 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$0.812 \quad$ (Dreisbach 1959) $0.7991 \quad$ (Riddick et al. 1986) 6.43, 2.37, $0.79 \quad\left(-137.05,-166.15,-127.95^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
52.96, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
32.9, $22.5\left(0,25^{\circ} \mathrm{C}\right.$, shake flask-GC, calculated-group contribution, Polak \& Lu 1973)
19.1* (shake flask-GC, measured range $25-149.5^{\circ} \mathrm{C}$, Price 1976)
11.0 (selected, Riddick et al. 1986)
21.0* (IUPAC tentative value, temp range $0-150^{\circ} \mathrm{C}$, Shaw 1989a)
18.67* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-422.7 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$28955^{*} \quad\left(23.10^{\circ} \mathrm{C}\right.$, ebulliometry, measured range: $14.256-58.789^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80983-1127.187 /\left(228.900+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $14.256-58.789^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)
31204* (calculated-Antoine eq. regression, temp range -63.6 to $58^{\circ} \mathrm{C}$, Stull 1947)
31280 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90983-1127.187 /\left(228.9+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -20 to $100^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
31277* (Antoine eq., temp range -34.9 to $81.3^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80983-1127.187 /\left(228.900+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -34.9 to $81.3^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7120.0 /(\mathrm{T} / \mathrm{K})]+7.536008$; temp range -63.6 to $225.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)

31280 (interpolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.594371-1132.099 /\left(229.494+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $14.256-58.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data of Willingham et al. 1945, Boublik et al. 1984)
32010 (interpolated-Antoine eq., temp range -35 to $81^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80983-1127.83 /\left(228.90+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -35 to $81^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 31300 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.93941-1129.73 /\left(229.215+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 31290 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.95181-1136.355 /(-43.159+\mathrm{T} / \mathrm{K})$; temp range $278-322 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=33.6319-2.5524 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.3142 \cdot \log (\mathrm{~T} / \mathrm{K})+1.4759 \times 10^{-10} .(\mathrm{T} / \mathrm{K})+3.914 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $145-500 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
130000 (recommended, Mackay \& Shiu 1981)
141000 (calculated-P/C, Mackay \& Shiu 1981)
131190 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.85 (shake flask, Hansch \& Leo 1979)
3.85 (calculated-fragment const., Valvani et al. 1981)
3.85 (recommended, Sangster 1989, 1993)
2.42; 2.63 (calculated-S, calculated-molar volume, Wang et al. 1992)
3.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Photooxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=5.16 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ correlated $)=4.49 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K , measured range 300-498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.0 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=5.50 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}}=5.50 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (abstraction mechanism, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=(5.67 \pm 0.29) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=(6.26 \pm 0.06) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{NO} 3}=4.06 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(5.90-0.23) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K , measured range $247-327 \mathrm{~K}$ (relative rate method, Harris \& Kerr 1988)
$\mathrm{k}_{\mathrm{OH}}=6.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=6.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with an estimated atmospheric lifetime of 22 h in air during summer daylight (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=6.30 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=4.06 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=19.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=4.06 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=(4.04-5.34) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (review, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=6.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=40.6 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=4.08 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ recommended $)=2.55 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}($ calc $)=2.55 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=5.78 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=4.40 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $6.30 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radicals and an estimated atmospheric lifetime of 22 h during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.6.1
Reported aqueous solubilities of 2,3-dimethylbutane at various temperatures

| Polak \& Lu 1973 |  | Price 1976 |  | Shaw 1989a |  | Ma̧czyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-GC/FID |  | IUPAC tentative values |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0 | 32.9 | 25 | 19.1 | 0 | 33 | 25 | 18.67 |
| 25 | 22.5 | 40.1 | 19.2 | 25 | 21 | 40.1 | 18.19 |
|  |  | 55.1 | 23.7 | 30 | 19 | 55.1 | 20.11 |
|  |  | 99.1 | 40.1 | 41 | 19 | 99.1 | 39.74 |
|  |  | 1213 | 56.8 | 50 | 21 | 121.3 | 67.03 |
|  |  | 137.3 | 97.9 | 70 | 28 | 137.3 | 100.5 |
|  |  | 149.5 | 171 | 90 | 35 | 149.5 | 138.8 |
|  |  |  |  | 110 | 46 |  |  |
|  |  |  |  | 130 | 75 |  |  |
|  |  |  |  | 150 | 180 |  |  |



FIGURE 2.1.1.1.6.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 2,3-dimethylbutane.

TABLE 2.1.1.1.6.2
Reported vapor pressures of 2,3-dimethylbutane at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{align*}
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)  \tag{2}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})  \tag{3}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{~T} / \mathrm{K}) \tag{4}
\end{align*}
$$

| Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | summary of literature data |  | selected values |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 14.256 | 19921 | -63.6 | 133.3 | -34.9 | 1333 | 57.988 | 101325 |
| 18.044 | 23451 | -44.5 | 666.6 | -24.3 | 2666 | 25.0 | 234.6 |
| 23.099 | 28955 | -34.9 | 1333 | -17.5 | 4000 |  |  |
| 27.746 | 34897 | -24.1 | 2666 | -12.5 | 5333 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 33.357 | 43320 | -12.4 | 5333 | -8.4 | 6666 | A | 6.80983 |
| 39.15 | 53654 | -4.9 | 7999 | -4.9 | 7999 | B | 1127.187 |
| 45.339 | 66756 | 5.40 | 13332 | 0.82 | 10666 | C | 228.900 |
| 52.06 | 83718 | 21.1 | 26664 | 5.34 | 13332 |  |  |
| 56.806 | 97604 | 39.0 | 53329 | 14.36 | 19998 | bp/ ${ }^{\circ} \mathrm{C}$ | 57.998 |
| 57.317 | 99201 | 58.0 | 101325 | 21.097 | 26664 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ | $\left.\mathrm{ol}^{-1}\right)=$ |
| 57.79 | 100693 |  |  | 26.588 | 33331 | at $25^{\circ} \mathrm{C}$ | 29.12 |
| 58.32 | 102390 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -128.2 | 31.257 | 39997 | at bp | 27.28 |
| 58.789 | 103907 |  |  | 38.982 | 53329 |  |  |
|  |  |  |  | 45.927 | 66661 |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 57.988 |  |  | 50.682 | 79993 |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | 55.404 | 93326 |  |  |
| A | 6.80983 |  |  | 56.283 | 95992 |  |  |
| B | 1127.187 |  |  | 57.145 | 98659 |  |  |
| C | 228.900 |  |  | 57.568 | 99992 |  |  |



FIGURE 2.1.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylbutane.

### 2.1.1.1.7 <br> 2,2,3-Trimethylbutane



Common Name: 2,2,3-Trimethylbutane
Synonym: triptene
Chemical Name: 2,2,3-trimethylbutane
CAS Registry No: 464-06-2
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right)_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-24.6 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 80.86 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.6901,0.6859 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959) 0.6901 (Weast 1984)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
145.2, $146.1\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 32.037, $28.94 \quad\left(25^{\circ} \mathrm{C}\right.$, at normal bp, Dreisbach 1959)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
2.259 (at mp, Dreisbach 1959; Chickos et al. 1999)
2.36, $2.2 \quad\left(-152.15,-25.45^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
28.53, 36.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
4.38 (estimated-nomograph of Kabadi \& Danner 1979; Brookman et al. 1985)
7.09 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$13840 \quad\left(25.3^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $12.6-81.8^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.79230-1200.563 /\left(226.650+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.6-81.8^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
13650 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.79230-1200.563 /\left(226.05+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-125^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
13652 (derived from compiled data, temp range $-18.8-205.94^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.79230-1200.563 /\left(226.050+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $-18.8-205.94^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
13650, 13660 (interpolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.92699-11206.087 /\left(226.731+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $22.7-105.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.92037-1202.337 /\left(226.256+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.6-81.77^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data of Forziati et al. 1949, Boublik et al. 1984)
13650 (interpolated-Antoine eq., temp range -19 to $106^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.79230-1200.563 /\left(226.05+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -19 to $106^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 ) 13650 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.9181-1201.098 /(-47.026+\mathrm{T} / \mathrm{K})$; temp range $284-355 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.18145-1390.726 /(-20.97+\mathrm{T} / \mathrm{K})$; temp range $353-483 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=32.3633-2.6614 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.7743 \cdot \log (\mathrm{~T} / \mathrm{K})-7.687 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+3.2006 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $249-531 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
241010 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=3.84 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ correlated $)=3.15 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 296 K , measured range 296-498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{OH}}=(3.6-5.05) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296-305 \mathrm{~K}$ (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=(4.21 \pm 0.08) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=5.23 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \mathrm{~K}, \mathrm{k}_{\mathrm{OH}}=4.09 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=4.23 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=2.23 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}(\mathrm{calc})=1.31 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=4.24 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}^{*}=2.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

### 2.1.1.1.8 <br> n-Pentane



Common Name: $n$-Pentane
Synonym: pentane
Chemical Name: n-pentane
CAS Registry No: 109-66-0
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{12} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{3} \mathrm{CH}_{3}$
Molecular Weight: 72.149
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ :
-129.67 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
36.06 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6262,0.6214 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 115.22, $116.1 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
26.42, $25.77 \quad\left(25^{\circ} \mathrm{C}\right.$ bp, Dreisbach 1959) 26.427, $25.786 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 8.393 (Dreisbach 1959; Riddick et al. 1986) 8.4 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 58.59, 63.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
360
120
38.5
49.7 (vapor saturation-GC, Barone et al. 1966)
$40.0 \quad$ (Baker 1967)
40.3* (shake flask-GC, measured range $4-30^{\circ} \mathrm{C}$, Nelson \& De Ligny 1968)
11.8* (shake flask-GC, measured range $5-35^{\circ} \mathrm{C}$, Pierotti \& Liabastre 1972)
65.7; 47.6, $44.6 \quad\left(0,25^{\circ} \mathrm{C}\right.$, shake flask-GC, calculated-group contribution, Polak \& Lu 1973)
39.5*
39.0 (shake flask-GC, Kryzanowska \& Szeliga 1978)
$40.0 \quad$ (partition coefficient, Rudakov \& Lutsyk 1979)
40.75 (generator column-GC, Tewari et al. 1982a)
$36.9 \quad$ (calculated-activity coeff. $\gamma$ and $\mathrm{K}_{\mathrm{OW}}$, Tewari 1982b)
40.6* (vapor saturation-GC, measured range $15-40^{\circ} \mathrm{C}$, Jönsson et al. 1982)
38.9 (shake flask-GC, Coates et al. 1985)
38.0 (selected, Riddick et al. 1986)
42.0* (IUPAC recommended best value, temp range $0-90^{\circ} \mathrm{C}$, Shaw 1989)
$\ln x=-333.59719+14358.472 /(\mathrm{T} / \mathrm{K})+47.97436 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature
calorimetric and solubility data, Tsonopoulos 1999)
44.09* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-422.7 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
68213* $\quad\left(24.828^{\circ} \mathrm{C}\right.$, static method, measured range -65 to $25^{\circ} \mathrm{C}$, Messerly \& Kennedy 1940)
$66760^{*} \quad\left(24.37^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $13.282-36.818^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87372-1075.816 /\left(233.369+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.282-36.818^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
71050* (interpolated-Antoine eq. regression, temp range -76.6 to $36.1^{\circ} \mathrm{C}$, Stull 1947)
68330 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85221-1064.63 /\left(232.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -35 to $80^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
68368* (interpolated- Antoine eq., temp range -50.14 to $57.53^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87632-1075.78 /\left(233.205+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -50.14 to $57.53^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 6595.1 /(\mathrm{T} / \mathrm{K})]+7.489673$; temp range -76.6 to $191^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$3400^{*} \quad\left(-30.86^{\circ} \mathrm{C}\right.$, gas saturation, measured range -129.54 to $-30.86^{\circ} \mathrm{C}$, Carruth \& Kobayashi 1973)
$57820^{*} \quad\left(20.57^{\circ} \mathrm{C}\right.$, ebulliometric method, measured range -4.4 to $68.218^{\circ} \mathrm{C}$, Osborn \& Douslin 1974)
68330 (interpolated-Antoine eq, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.12545-1132.518 /\left(239.074+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -65.2 to $24.83^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.96982-1060.916 /\left(231.577+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.28-36.82^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.99028-1071.187 /\left(232.766+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -4.4 to $68.21^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Osborn \& Douslin 1974, Boublik et al. 1984)
70915 (interpolated-Antoine eq., temp range -50 to $58^{\circ} \mathrm{C}$, Dean 1985. 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85296-1064.84 /\left(233.01+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -50 to $58^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
69810, 68880, 68330 (headspace-GC, correlated, Antoine eq., Hussam \& Carr 1985)
68330 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.97786-1064.84 /\left(232.012+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
68355 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.6922-1686.65 /(\mathrm{T} / \mathrm{K})$; temp range $143-233 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99466-1073.139 /(-40.188+\mathrm{T} / \mathrm{K})$; temp range $223-352 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.98799-1070.14 /(-40.485+\mathrm{T} / \mathrm{K})$; temp range $269-335 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.28417-1260.973 /(-14.031+\mathrm{T} / \mathrm{K})$; temp range $350-422 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.47436-2414.137 /(141.919+\mathrm{T} / \mathrm{K})$; temp range $418-470 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
68340* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{2.73425-1.988544 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+2.408406 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=309.209 \mathrm{~K}($ Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=33.3239-2.4227 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.2354 \cdot \log (\mathrm{~T} / \mathrm{K})+9.0199 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+4.105 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $143-470 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
127050 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
115900, 33430 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
128000 (calculated-P/C, Mackay \& Shiu 1975, 1990; Bobra et al. 1979; Mackay et al. 1979; Mackay 1981) 125000 (recommended, Mackay \& Shiu 1981)
128000, 125000, 123000, 122200, 10370 (calculated-P/C, Mackay \& Shiu 1981)
$78050,99075,126800,144020,174480\left(14.8,20.05,25.1,30.1,34.92^{\circ} \mathrm{C}\right.$, equilibrium cell-concentration ratioGC, Jönsson et al. 1982)
121410* (calculated-temp dependence eq. derived from exptl data, measured range $15-35^{\circ} \mathrm{C}$. Jönsson et al. 1982)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=19237.8 /(\mathrm{T} / \mathrm{K})+53.671 \cdot \ln (\mathrm{~T} / \mathrm{K})-372.214$; temp range: $15-35^{\circ} \mathrm{C}$ (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)
127670 (selected, Mills et al. 1982)
120970 (calculated-P/C, Eastcott et al. 1988)
100980 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
128050 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.50 (shake flask-GC, Hansch et al. 1968)
3.39 (shake flask-GC, Leo et al. 1975)
2.99, 3.42, 3.48 (calculated-fragment const., Rekker 1977)
3.23 (Hansch \& Leo 1979)
3.64 (calculated-activity coeff. $\gamma$, Wasik et al. 1981,1982)
3.62 (generator column-GC, Tewari et al. 1982a,b)
2.37 (HPLC-k' correlation, Coates et al. 1985)
3.62, 3.60 (generator column-GC, calculated-activity coeff. $\gamma$, Schantz \& Martire 1987)
3.45 (recommended, Sangster 1989, 1993)
3.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
2.05* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\circ}$ in octanol, measured range $20.29-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997) 1.95 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=5.8 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=(3.74 \pm 0.13) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=5.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}}=5.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=5.8 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ room temp. (abstraction mechanism, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=4.13 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a)
$\mathrm{k}_{\mathrm{NO} 3}=(8.1 \pm 1.7) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1984a; Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=(4.13 \pm 0.08) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=4.06 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson 1986; quoted, Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}=4.29 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in Smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=3.94 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991)
$\mathrm{k}_{\mathrm{OH}}=4.06 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=8.0 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=8.1 \times 10^{-17} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=3.94 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K with summer daylight atmospheric lifetime $\tau=35 \mathrm{~h}$ (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}} *=3.94 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=9.0 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=8.2 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=7.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=4.00 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=8.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=3.70 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $230-400 \mathrm{~K}$ (relative rate method, DeMore \& Bayes 1999)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $3.94 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical and an estimated atmospheric lifetime $\tau=35 \mathrm{~h}$ (Altshuller 1990).

TABLE 2.1.1.1.8.1
Reported aqueous solubilities of $n$-pentane at various temperatures
1.

| Nelson \& De Ligny 1968 |  | Pierotti \& Liabastre 1972 |  | Polak \& Lu 1973 |  | Price 1976 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-GC |  | shake flask-GC |  | shake flask-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 4.0 | 40.9 | 5.11 | 10.94 | 0 | 65.7 | 25 | 39.6 |
| 10 | 42.9 | 15.21 | 11.80 | 25 | 47.6 | 40.1 | 39.8 |
| 20 | 39.3 | 25.11 | 11.20 |  |  | 55.7 | 41.8 |
| 25 | 40.5 | 35.21 | 10.89 |  |  | 99.1 | 69.4 |
| 30 | 40.5 |  |  |  |  | 121.3 | 110 |
|  |  |  |  |  |  | 137.3 | 210 |
|  |  |  |  |  |  | 149.5 | 298 |

2. 

| Jonsson et al. 1982 |  | Shaw 1989a |  | Ma̧czyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| vapor saturation-GC |  | IUPAC recommended |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 15 | 42.9 | 0 | 66 | 0 | 56.12 |
| 20 | 41.4 | 10 | 43 | 4 | 52.11 |
| 25 | 40.6 | 20 | 40 | 10 | 48.1 |
| 30 | 40.3 | 25 | 42 | 15 | 48.1 |
| 40 | 40.6 | 30 | 41 | 20 | 44.09 |
|  |  | 40 | 40 | 25 | 44.09 |
|  |  | 50 | 41 | 30 | 44.09 |
|  |  | 60 | 43 | 35.1 | 44.09 |
|  |  | 70 | 46 | 40.1 | 44.09 |
|  |  | 80 | 50 | 55.7 | 48.1 |
|  |  | 90 | 58 | 99.1 | 88.18 |
|  |  | 110 | 86 | 121.3 | 136.3 |
|  |  | 130 | 150 | 137.3 | 192.4 |
|  |  | 150 | 300 | 149.5 | 260.5 |



FIGURE 2.1.1.1.8.1 Logarithm of mole fraction solubility $(\ln x)$ versus reciprocal temperature for $n$-pentane.

## TABLE 2.1.1.1.8.2

Reported vapor pressures of n-pentane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
(3)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4)
$\log \left(\mathrm{P} / \mathrm{P}_{\Phi}\right)=\mathrm{A}[1-\Phi /(\mathrm{T} / \mathrm{K})]$
(5) where $\log \mathrm{A}=\mathrm{a}+\mathrm{b}(\mathrm{T} / \mathrm{K})+\mathrm{c}(\mathrm{T} / \mathrm{K})^{2}$ - Cox eq. I
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{0} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{0} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{\mathrm{A}_{0}-\mathrm{A}_{1} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{A}_{2} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$
(6) $\quad-$ Cox eq. II
1.

| Messerly \& Kennedy 1940 |  | Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static method-manometer |  | ebulliometry |  | summary of literature data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| -65.178 | 411 | 13.282 | 43322 | -76.6 | 133.3 | -50.14 | 1333 |
| -48.811 | 1604 | 18.647 | 53657 | -62.5 | 666.6 | -40.25 | 2666 |
| -39.537 | 2818 | 24.371 | 66756 | -50.1 | 1333 | -33.86 | 4000 |
| -27.420 | 5951 | 30.592 | 83719 | -40.1 | 2666 | -29.24 | 5333 |
| -17.476 | 10340 | 34.981 | 97604 | -29.2 | 5333 | -25.42 | 6666 |
| -9.793 | 15341 | 35.453 | 99201 | -22.2 | 7999 | -22.19 | 7999 |
| -2.359 | 21933 | 35.89 | 100694 | -12.6 | 13332 | -16.98 | 10666 |
| 3.618 | 28767 | 36.379 | 102393 | 1.9 | 26664 | -12.59 | 13332 |
| 9.621 | 37303 | 36.818 | 103911 | 18.5 | 53329 | -4.33 | 19998 |
| 14.653 | 45947 |  |  | 36.1 | 101325 | 1.92 | 26664 |
| 18.613 | 53773 | bp/ ${ }^{\circ} \mathrm{C}$ | 36.073 |  |  | 7.01 | 33331 |
| 21.679 | 60539 |  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -129.7 | 11.34 | 39997 |

(Continued)

TABLE 2.1.1.1.8.2 (Continued)

2.

Carruth \& Kobayashi 1973



FIGURE 2.1.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-pentane.

TABLE 2.1.1.1.8.3
Reported Henry's law constants and octanol-air partition coefficients of $n$-pentane at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

$$
\begin{equation*}
\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{~T} / \mathrm{K})^{2} \tag{4}
\end{equation*}
$$

| Henry's law constant | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {OA }}$ |
| :---: | :---: |
| Jönsson et al. 1982 | Gruber et al. 1997 |
| equilibrium cell-GC | GC det'd activity coefficient |
| $t /{ }^{\circ} \mathrm{C} \quad \mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ | $t /{ }^{\circ} \mathrm{C} \quad \quad \log \mathrm{K}_{\text {OA }}$ |
| 15.0 78035\# | 20.292 .053 |
| 15.1 77905 | 30.3 1.911 |
| 15.1 77905 | $40.4 \quad 1.781$ |
| 20.0 98674 | 50.28 1.670 |
| 20 100713\# |  |
| 2097490 |  |
| 25.0 121511 |  |
| $25 \quad 125828$ |  |
| $25 \quad 127774$ |  |
| 30.0 146533\# |  |
| $30 \quad 144022$ |  |
| 35.0 173105\# |  |
| 35175477 |  |
| \# interpolated from exptl data |  |



FIGURE 2.1.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for $n$-pentane.


FIGURE 2.1.1.1.8.4 Logarithm of $\mathrm{K}_{\mathrm{OA}}$ versus reciprocal temperature for $n$-pentane.

### 2.1.1.1.9 2-Methylpentane (Isohexane)



Common Name: 2-Methylpentane
Synonym: isohexane
Chemical Name: 2-methylpentane
CAS Registry No: 107-83-5
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{14} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{3}$
Molecular Weight: 86.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -153.6 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 60.26 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6322,0.6485\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 136.31, $132.88\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 29.87, 27.79 ( $25^{\circ} \mathrm{C}$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
6.203 (Dreisbach 1959)
6.268 (Riddick et al. 1986) 6.27 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : $52.43,50.6$ (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
13.8 (shake flask-GC, McAuliffe 1963, 1966)
16.21 (vapor saturation-GC, Barone et al. 1966)
19.45; 15.7, $15.6 \quad\left(0,25^{\circ} \mathrm{C}\right.$, shake flask-GC, calculated-group contribution, Polak \& Lu 1973)
14.2 (shake flask-GC, Leinonen \& Mackay 1973)
13.0* (shake flask-GC, measured range $25-149.5^{\circ} \mathrm{C}$, Price 1976)
13.7* (recommended best value, temp range $25-150^{\circ} \mathrm{C}$, IUPAC Solubility Data Series, Shaw 1989a)
13.88* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-422.7 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
29040* $\quad\left(25.64^{\circ} \mathrm{C}\right.$, ebulliometry, measured temp range $12.758-61.066^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83910-1135.410 /\left(226.572+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.758-61.066^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
27820* (calculated-Antoine eq. regression, temp range -60 to $60.3^{\circ} \mathrm{C}$, Stull 1947)
28240 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83910-1135.410 /\left(226.572+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -15 to $100^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
28238; 28200* (derived from compiled, interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83910-1135.410 /\left(226.572+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -32.1 to $83.4^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
27780 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7676.6 /(\mathrm{T} / \mathrm{K})]+7.944630$; temp range: -60.9 to $60.3^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
28240 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.86839-1151.401 /\left(228.477+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.78-61^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
28230 (interpolated-Antoine eq., temp range -32 to $83^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83910-1135.41 /\left(226.57+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -32 to $83^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
28300 (selected lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.98850-1148.74 /\left(228.166+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 28250 (calculated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.97783-1142.922 /(-45.657+\mathrm{T} / \mathrm{K})$; temp range $293-335 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=30.7477-2.4888 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.2295 \cdot \log (\mathrm{~T} / \mathrm{K})-2.3723 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.2402 \times 10^{-6}$.
$(\mathrm{T} / \mathrm{K})^{2}$; temp range $120-498 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$72190 \quad\left(50^{\circ} \mathrm{C}\right.$, vapor-liquid equilibria VLE data, Horstmann et al. 2004)
$\log (\mathrm{P} / \mathrm{kPa})=5.99313-1151.40 /(\mathrm{T} / \mathrm{K}-44.673)$; temp range not specified (Antoine eq., Horstmann et al. 2004)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):

| 170000 | (recommended; Mackay \& Shiu 1981) |
| :--- | :--- |
| 175490 | (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975) |
| 196800,49430 | (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 176160 | (calculated-P/C, Eastcott et al. 1988) |
| $83590^{*}$ | (EPICS-GC, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988) |
| $\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=2.959-957.2 /(\mathrm{T} / \mathrm{K}) ;$ temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988) |  |
| 176280 | $(\mathrm{calculated}-$ vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |
| 746 | $\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001) |
| $\log \mathrm{K}_{\mathrm{AW}}=2.470-288 /(\mathrm{T} / \mathrm{K})($ summary of literature data, Staudinger \& Roberts 2001) |  |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
2.80 (calculated $\pi$ constant, Hansch et al. 1968)
2.85 (calculated-MCI $\chi$, Murray et al. 1975)
3.23 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.74 (calculated-fragment constant, Müller \& Klein 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=(3.2 \pm 0.6) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976, Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(5.68 \pm 0.24) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=5.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=9.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=5.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, estimated atmospheric lifetime was 25 h during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}(\operatorname{exptl})=1.71 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}(\mathrm{calc})=1.83 \times 10^{-16} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}=5.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.8 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: half-life of $2.4-24 \mathrm{~h}$ based on photooxidation rate constant of $3.2 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the gas-phase reaction with hydroxyl radical (Darnall et al. 1976);
atmospheric lifetime was estimated to be 25 h during summer daylight, based on photooxidation rate constant of $5.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with hydroxyl radical in air (Altshuller 1991).

## TABLE 2.1.1.1.9.1

Reported aqueous solubilities of 2-methylpentane at various temperatures

| Polak \& Lu 1973 |  | Price 1976 |  | Shaw 1989a |  | Ma̧czyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-GC |  | IUPAC recommended |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0 | 19.45 | 25 | 13 | 25 | 13.7 | 0 | 18.19 |
| 25 | 15.7 | 40.1 | 13.8 | 30 | 13 | 25 | 13.88 |
|  |  | 55.7 | 15.7 | 40 | 14 | 40 | 13.88 |
|  |  | 99.1 | 27.1 | 50 | 15 | 55.7 | 15.32 |
|  |  | 118 | 44.9 | 70 | 17 | 99.1 | 30.64 |
|  |  | 137.3 | 86.8 | 90 | 23 | 118 | 46.92 |
|  |  | 149.5 | 113 | 110 | 36 | 137.3 | 76.6 |
|  |  |  |  | 130 | 68 | 145.9 | 110.12 |
|  |  |  |  | 150 | 120 |  |  |



FIGURE 2.1.1.1.9.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 2-methylpentane.

TABLE 2.1.1.1.9.2
Reported vapor pressures and Henry's law constants of 2-methylpentane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1a) |
| :--- | :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t}^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2a) |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3a) |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$ | (5) |  |  |


| Vapor pressure |  |  |  |  |  | Henry's law constant <br> Ashworth et al. 1988 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Willin | al. 1945 |  |  | Zwolinski | ilhoit 1971 |  |  |
| ebulliometry |  | summary of literature data |  | selected values |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 12.758 | 16620 | -60.9 | 133.3 | -32.1 | 1333 | 10 | 70624 |
| 16.82 | 19921 | -41.7 | 666.6 | -21.6 | 2666 | 15 | 70320 |
| 20.584 | 23451 | -32.1 | 1333 | -14.8 | 4000 | 20 | 89470 |
| 25.617 | 29038 | -214 | 2666 | -9.8 | 5333 | 25 | 83593 |
| 30.237 | 34896 | -9.7 | 5333 | -5.7 | 6666 | 30 | 85924 |
| 35.810 | 43322 | -1.9 | 7999 | -2.2 | 7999 |  |  |
| 41.507 | 53656 | 8.1 | 13332 | 3.45 | 10666 |  | A -B/(T/K) |
| 47.714 | 66757 | 24.1 | 26664 | 8.06 | 13332 |  | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ |
| 54.388 | 83718 | 41.5 | 53329 | 16.92 | 19998 | A | 2.959 |
| 59.099 | 97605 | 60.3 | 101325 | 23.624 | 26664 | B | 957.2 |
| 59.607 | 99204 |  |  | 29.084 | 33331 |  |  |
| 60.074 | 100694 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -154 | 33.724 | 39997 |  |  |
| 60.602 | 102394 |  |  | 41.40 | 53329 |  |  |
| 61.066 | 103913 |  |  | 47.672 | 66661 |  |  |
|  |  |  |  | 53.020 | 79993 |  |  |
| bp/ $/{ }^{\circ} \mathrm{C}$ | 60.271 |  |  | 57.706 | 93326 |  |  |
|  |  |  |  | 58.579 | 95992 |  |  |
| eq. 2 | P/mmHg |  |  | 59.434 | 98659 |  |  |
| A | 6.93910 |  |  | 60.271 | 101325 |  |  |
| B | 1135.410 |  |  | 25.0 | 28238 |  |  |
| C | 226.572 |  |  |  |  |  |  |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  |  |  | A | 6.83910 |  |  |
|  |  |  |  | B | 1135.410 |  |  |
|  |  |  |  | C | 226.572 |  |  |
|  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 60.271 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /$ | $\left.\mathrm{ol}^{-1}\right)=$ |  |  |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 29.76 |  |  |
|  |  |  |  | at bp | 27.79 |  |  |



FIGURE 2.1.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpentane.


FIGURE 2.1.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-methylpentane.

### 2.1.1.1.10



Common Name: 3-Methylpentane
Synonym: diethylmethylmethane
Chemical Name: 3-methylpentane
CAS Registry No: 96-14-0
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{14} ; \mathrm{CH}_{3} \mathrm{CH}_{2}\left(\mathrm{CH}_{3}\right) \mathrm{CHCH}_{2} \mathrm{CH}_{3}$
Molecular Weight: 86.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-162.9 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
63.27 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $25^{\circ} \mathrm{C}$ ):
$0.66431,0.65976\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ :
129.7, $130.6\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
$129.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$30.28,28.08\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$5.035 \quad$ (Riddick et al. 1986)
5.31 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
48.17, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
12.8 (shake flask-GC, McAuliffe 1966)
21.5; 17.9, $17.2\left(0 ; 25^{\circ} \mathrm{C}\right.$, shake flask-GC, calculated-group contribution, Polak \& Lu 1973)
13.1 (shake flask-GC, Price 1976)
12.9 (partition coefficient-GC, Rudakov \& Lutsyk 1979)
13.0 (selected, Riddick et al. 1986)
12.9 (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)
22.02, $16.76\left(0,25^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
$29040 \quad\left(23.2^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $15.29-64.083^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84887-1152.368 /\left(227.129+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $15.29-64.083^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
24970 (Antoine eq. regression, temp range -59 to $63.3^{\circ} \mathrm{C}$, Stull 1947)
25300 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84887-1152.368 /\left(227.129+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ) ; temp range -15 to $105^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
25305, 25300 (derived from compiled data, interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84887-1152.368 /\left(227.129+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -30.1 to $86.6^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
24940 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7743.9 /(\mathrm{T} / \mathrm{K})]+7.947042$; temp range -59 to $63.3^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)

```
25310 (interpolated-Antoine eq, Boublik et al. 1984)
\(\log (\mathrm{P} / \mathrm{kPa})=6.36895-1997.558 /\left(202.608+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\); temp range \(69.2-271.1^{\circ} \mathrm{C}\) (Antoine eq. from reported exptl.
    data, Boublik et al. 1984)
25300 (interpolated-Antoine eq., temp range -30 to \(87^{\circ} \mathrm{C}\), Dean 1985 , 1992)
\(\log (\mathrm{P} / \mathrm{mmHg})=6.84887-1152.368 /\left(227.13+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\); temp range -30 to \(87^{\circ} \mathrm{C}\) (Antoine eq., Dean 1985,1992 )
25300 (lit. average, Riddick et al. 1986)
\(\log (\mathrm{P} / \mathrm{kPa})=5.98356-11133.52 /\left(224.944+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\); temp range not specified (Antoine eq., Riddick et al. 1986)
25320 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.97897-1155.28 /(-45.659+\mathrm{T} / \mathrm{K})\); temp range 293-338 K (Antoine eq., Stephenson \&
    Malanowski 1987)
\(\log (\mathrm{P} / \mathrm{mmHg})=35.2848-2.6773 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.8546 \cdot \log (\mathrm{~T} / \mathrm{K})+2.2352 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+4.0277 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;\)
    temp range \(110-504 \mathrm{~K}\) (vapor pressure eq., Yaws 1994)
```

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 172000 | (recommended; Mackay \& Shiu 1981) |
| :--- | :--- |
| 171490 | (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975) |
| 196800,49430 | (calculated-contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 170210 | (calculated-P/C, Eastcott et al. 1988) |
| 139390 | (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988) |
| 113670 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :

| 2.80 | (calculated- $\pi$ const., Hansch et al. 1968; Hansch \& Leo 1979) |
| :--- | :--- |
| 2.88 | (calculated-MCI $\chi$, Murray et al. 1975) |
| 3.81 | (calculated-intrinsic molar volume $\mathrm{V}_{\mathrm{I}}$ and solvatochromic parameters, Leahy 1986) |
| $3.60 \pm 0.20$ | (recommended, Sangster 1989) |
| 3.18 | (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992) |
| 3.74 | (calculated-fragment constant, Müller \& Klein 1992) |
| 2.9168 | (calculated-UNIFAC group contribution, Chen et al. 1993) |
| 3.60 | (recommended, Sangster 1993) |

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=1.28 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Greiner 1967; quoted, Altshuller \& Bufalini 1971)
$\mathrm{k}_{\mathrm{OH}}=(4.3 \pm 0.9) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=6.82 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at atmospheric pressure and 305 K (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=(5.78 \pm 0.11) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)
$\mathrm{k}_{\mathrm{OH}}=5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , estimated atmospheric lifetime 25 h , during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=2.04 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=2.53 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}=5.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}^{*}=2.2 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $4.30 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical with half-life of 2.4-24 h (Darnall et al. 1976; Lloyd et al. 1976);
rate constant of $5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \cdot \mathrm{~s}^{-1}$ for the reaction with OH radical with an estimated atmospheric lifetime of 25 h during summer daylight (Altshuller 1991).

### 2.1.1.1.11 <br> 2,2-Dimethylpentane



Common Name: 2,2-Dimethylpentane
Synonym:
Chemical Name: 2,2-dimethylpentane
CAS Registry No: 590-35-2
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16} ; \mathrm{CH}_{3} \mathrm{C}\left(\mathrm{CH}_{3}\right)_{2} \mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{3}$
Molecular Weight: 100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-123.7 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
79.2 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.6739 \quad$ (Weast 1984) $0.6739,0.6695 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$148.69 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
5.812 (Dreisbach 1959)
5.86 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
39.55, 49.74 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

```
4.40 (shake flask-GC, Price 1976)
4.90 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)
```

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$13824 \quad\left(24.67^{\circ} \mathrm{C}\right.$, manometer, measured range $15.325-80.05^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81509-1190.298 /\left(223.343+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.325-80.05^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer measurements, Willingham et al. 1945)
$13850 \quad\left(24.708^{\circ} \mathrm{C}\right.$, ebulliometry, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81479-1190.033 /\left(223.303+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.188-80.074{ }^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
14030 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81480-1190.033 /\left(223.303+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-115^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
14026 (interpolated-Antoine eq., temp range -18.6 to $103.75^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81480-1190.033 /\left(223.303+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -18.6 to $103.75^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
13500 (interpolated-Antoine eq., temp range -69.3 to $49.7^{\circ} \mathrm{C}$, Weast $1972-72$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7271.0 /(\mathrm{T} / \mathrm{K})]+7.841340$; temp range -69.3 to $49.7^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
14030 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.93788-1189.09 /\left(223.198+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.32-80.05^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
14030 (interpolated-Antoine eq., temp range -18 to $103^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84180-1190.033 /\left(223.3+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -18 to $103^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
14010 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93117-1185.576 /(-50.37+\mathrm{T} / \mathrm{K})$; temp range $277-354 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.2280-1399.333 /(-20.934+\mathrm{T} / \mathrm{K})$; temp range $353-483 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=6.2875-2.1682 \times 10^{3} /(\mathrm{T} / \mathrm{K})+2.6936 \cdot \log (\mathrm{~T} / \mathrm{K})-1.5525 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.0917 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $149-527 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
318000 (calculated-P/C, Mackay \& Shiu 1981)
319200 (selected, Mills et al. 1982)
319420 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.10 (calculated $-\pi$ substituent constant, Hansch et al. 1968)
3.62 (calculated $-\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
4.14 (calculated-fragment constant, Müller \& Klein 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(2.66 \pm 0.08) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=3.37 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=3.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=9.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990) $\mathrm{k}_{\mathrm{OH}}=3.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

### 2.1.1.1.12

2,4-Dimethylpentane


Common Name: 2,4-Dimethylpentane
Synonym: diisopropylmethane
Chemical Name: 2,4-dimethylpentane
CAS Registry No: 108-08-7
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{3}$
Molecular Weight: 100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-119.5 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 80.49 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6727,0.6683 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 148.95, $149.9 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 32.89, $29.501 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
6.840 (Dreisbach 1959)
6.845 (Riddick et al. 1986) 6.85 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
44.46, 44.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
3.62 (shake flask-GC, McAuliffe 1963)
4.06 (shake flask-GC, McAuliffe 1966; quoted, Hermann 1972; Price 1976)
6.50; $5.50 \quad\left(0 ; 25^{\circ} \mathrm{C}\right.$, shake flask-GC, Polak \& Lu 1973)
4.41 (shake flask-GC, Price 1976)
4.20 (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)
6.12, $4.45 \quad\left(0,25^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
12635 (Antoine eq. regression, temp range -48 to $80.5^{\circ} \mathrm{C}$, Stull 1947)
$11730 \quad\left(22.54^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $13.714-81.374^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82621-1192.041 /\left(221.634+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.714-81.374^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Forziati et al. 1949)
13120 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82621-1192.041 /\left(221.634+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-115^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
13119 (interpolated-Antoine eq, temp range -17.0 to $104.94^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82621-1192.041 /\left(221.634+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -17.0 to $104.94^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
12620 (interpolated-Antoine eq., temp range -48.0 to $80.5^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8167.4 /(\mathrm{T} / \mathrm{K})]+7.961374$; temp range -48.0 to $80.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
13120 (interpolated-Antoine eq., temp range $13.7-81.37^{\circ} \mathrm{C}$, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.95675-1195.154 /\left(221.992+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.7-81.37^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

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15450 (interpolated-Antoine eq., temp range -17 to 105 C
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13000 (selected, Riddick et al. 1986)
log}(\textrm{P}/\textrm{kPa})=5.94917-1191.06/(221.540 + t/ / C ); temp range not specified (Antoine eq., Riddick et al. 1986)
13125 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log}(\mp@subsup{\textrm{P}}{\textrm{L}}{}/\textrm{kPa})=5.95921-1196.516/(-50.993 + T/K); temp range 284-355 K (Antoine eq., Stephenson & Malanowski
    1987)
log}(\textrm{P}/\textrm{mmHg})=35.9436-2.846\times1\mp@subsup{0}{}{3}/(\textrm{T}/\textrm{K})-9.9938\cdot\operatorname{log}(\textrm{T}/\textrm{K})+8.0613\times1\mp@subsup{0}{}{-11}.(\textrm{T}/\textrm{K})+3.6419\times1\mp@subsup{0}{}{-6}.(\textrm{T}/\textrm{K}\mp@subsup{)}{}{2}
    temp range 154-520 K (vapor pressure eq., Yaws 1994)
Henry's Law Constant ( \(\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
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319300 (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
326600, 73120 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
$300000 \quad$ (recommended; Mackay \& Shiu 1981)
297300 (calculated-P/C, Eastcott et al. 1988)
160050 (calculated-molecular connectivity index MCI $\chi$, Nirmalakhandan \& Speece 1988)
298050 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.10 (calculated $-\pi$ constant, Hansch et al. 1968)
3.17 (calculated-MCI $\chi$, Murray et al. 1975)
3.66 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
4.14 (calculated-f constant, Müller \& Klein 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(5.26 \pm 0.11) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984 c )
$\mathrm{k}_{\mathrm{OH}}=5.10 \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=1.44 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=2.89 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}=5.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3} *=1.5 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $5.10 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radicals and an estimated lifetime of 27 h during summer daylight (Altshuller 1991).

### 2.1.1.1.13 <br> 3,3-Dimethylpentane



Common Name: 3,3-Dimethylpentane
Synonym:
Chemical Name: 3,3-dimethylpentane
CAS Registry No: 562-49-2
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16} ; \mathrm{CH}_{3} \mathrm{CH}_{2}\left(\mathrm{CH}_{3}\right)_{2} \mathrm{CH}_{2} \mathrm{CH}_{3}$
Molecular Weight: 100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-134.4 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
86.06 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.6933,0.6891 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$144.5 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
33.02, $29.74 \quad\left(25^{\circ} \mathrm{C}\right.$, normal bp, Dreisbach 1959)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
7.067 (Dreisbach 1959)
7.07 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
51.16, 49.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
5.94* (shake flask-GC, measured range $25-150.4^{\circ} \mathrm{C}$, Price 1976)
6.68* (calculated-liquid-liquid equilibrium LLE data, temp range 298.2-423.2 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
10600* (Antoine eq. regression, temp range -45.9 to $86.1^{\circ} \mathrm{C}$ Stull 1947)
10316* $\quad\left(23.521^{\circ} \mathrm{C}\right.$, ebulliometry, measured range -13.5 to $82^{\circ} \mathrm{C}$ Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82668-1228.063 /\left(225.316+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.484-80.962^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
11044 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82667-1228.663 /\left(225.316+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $5-130^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
11039* (interpolated-Antoine eq., temp range -14.4 to $111.25^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82667-1228.663 /\left(225.316+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -14.4 to $111.25^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
10600 (interpolated-Antoine eq., temp range -45.9 to $86.1^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8145.4 /(\mathrm{T} / \mathrm{K})]+7.869254$; temp range -45.9 to $86.1^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
11045 (interpolated-Antoine eq., temp range $13.484-86.96^{\circ} \mathrm{C}$, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.95327-1229.625 /\left(225.427+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.484-86.96^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
11045 (interpolated-Antoine eq., temp range -14 to $112^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82667-1228.663 /\left(225.32+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -14 to $112^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$ 11150, 11040 (interpolated-Antoine eq.-I, III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.95139-1228.138 /(-47.819+\mathrm{T} / \mathrm{K})$; temp range $285-360 \mathrm{~K}$ (Antoine eq. -I , Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.35011-1415.316 /(-31.302+\mathrm{T} / \mathrm{K})$; temp range $213-281 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.94685-1225.973 /(-48.144+\mathrm{T} / \mathrm{K})$; temp range $280-360 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=30.2570-2.6313 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.9839 \cdot \log (\mathrm{~T} / \mathrm{K})+4.6848 \times 10^{-13} \cdot(\mathrm{~T} / \mathrm{K})+2.717 \times 10^{-6}$. $(\mathrm{T} / \mathrm{K})^{2}$; temp range $139-536 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
186000 (calculated-P/C, Mackay \& Shiu 1981)
186305 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 2.1.1.1.13.1
Reported aqueous solubilities of 3,3-dimethylpentane at various temperatures

| Price $\mathbf{1 9 7 6}$ |  |  | Ma̧czyński et al. $\mathbf{2 0 0 4}$ |  |
| :--- | :---: | :---: | :---: | :---: |
|  | shake flask-GC |  | calc-recommended LLE data |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{\mathbf{- 3}}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 25 | 5.92 |  | 25 | 6.68 |
| 40.1 | 6.78 |  | 40 | 6.68 |
| 55.7 | 8.17 |  | 56 | 7.79 |
| 69.7 | 10.3 |  | 70 | 8.91 |
| 99.1 | 15.8 |  | 99 | 16.14 |
| 118 | 27.3 |  | 118 | 26.17 |
| 140.4 | 67.3 |  | 150 | 66.81 |
| 150.4 | 86.1 |  |  |  |



FIGURE 2.1.1.1.13.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 3,3-dimethylpentane.

## TABLE 2.1.1.1.13.2

Reported vapor pressures of 3,3-dimethylpentane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$ | (5) |  |


| Stull 1947 |  | Forziati et al. 1949 |  |  |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  |  |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  | set 1 |  | set 2 |  |  |  |
| -45.9 | 133.3 | 13.443 | 6383 | 17.163 | 7658 | -14.41 | 1333 |
| -25.0 | 666.6 | 17.231 | 7677 | 20.484 | 8969 | -2.96 | 2666 |
| -14.4 | 1333 | 30.533 | 8985 | 34.355 | 16623 | 4.36 | 4000 |
| -2.90 | 2666 | 23.521 | 10316 | 38.804 | 19926 | 9.852 | 5333 |
| 9.90 | 5333 | 26.318 | 11704 | 53.385 | 34902 | 14.297 | 6666 |
| 18.1 | 7999 | 30.086 | 13826 | 59.444 | 43327 | 18.055 | 7999 |
| 29.3 | 13332 | 34.406 | 16613 | 84.792 | 976-7 | 24.231 | 10666 |
| 46.2 | 26664 | 38.790 | 19917 | 85.344 | 99201 | 29.241 | 13332 |
| 65.5 | 53329 | 48.72 | 23438 | 85.854 | 100696 | 38.880 | 19998 |
| 86.1 | 101325 | 48.34 | 28954 | 86.429 | 102396 | 46.173 | 26664 |
|  |  | 53.37 | 34893 |  |  | 52.114 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -135 | 59.44 | 43322 |  |  | 57.164 | 39997 |
|  |  | 65.697 | 53645 |  |  | 65.519 | 53329 |
|  |  | 72.384 | 66733 |  |  | 72.347 | 66661 |
|  |  | 79.651 | 83682 |  |  | 78.168 | 79993 |
|  |  | 84.78 | 97575 | bp/ ${ }^{\circ} \mathrm{C}$ | 86.069 | 83.272 | 93326 |
|  |  | 85.335 | 99206 |  |  | 84.222 | 95992 |

TABLE 2.1.1.1.13.2 (Continued)



FIGURE 2.1.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 3,3-dimethylpentane.

### 2.1.1.1.14 <br> 2,2,4-Trimethylpentane (Isooctane)



Common Name: 2,2,4-Trimethylpentane
Synonym: isooctane, isobutyltrimethylmethane
Chemical Name: 2,2,4-trimethylpentane
CAS Registry No: 504-84-1
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{18} ; \mathrm{CH}_{3} \mathrm{C}\left(\mathrm{CH}_{3}\right)_{2} \mathrm{CH}_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{3}$
Molecular Weight: 114.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -107.30 (Stull 1947; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 99.22 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6919,0.6878 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $165.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987) 185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 36.92, $32.01 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.196 (Riddick et al. 1986) 9.27 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 55.52, 43.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
2.44 (shake flask-GC, McAuliffe 1963,1966)
2.46; $2.05 \quad\left(0 ; 25^{\circ} \mathrm{C}\right.$, shake flask-GC, Polak \& Lu 1973)
1.14 (shake flask-GC, Price 1976)
2.50, 2.0, 2.20 $\quad\left(0,20,25^{\circ} \mathrm{C}\right.$, IUPAC recommended values, Shaw 1989b)
2.30, 1.65, 1.65 (0.20, $25^{\circ} \mathrm{C}$, calculated-liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$6371 \quad\left(24.4^{\circ} \mathrm{C}\right.$, ebulliometry, measured temp range $24.4-100.13^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81189-1257.840 /\left(220.735+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $24.4-100.13^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Willingham et al. 1945)
6250 (calculated-Antoine eq. regression, temp range -36.4 to $99^{\circ} \mathrm{C}$, Stull 1947)
$1739,6573,19528\left(0,25,50^{\circ} \mathrm{C}\right.$, static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)
6580 (calculated from determined data, Dreisbach 1959; quoted, Hine \& Mookerjee 1975)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81189-1257.840 /\left(220.735+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15-120^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
6573 (interpolated-Antoine eq., temp range -4.3 to $125.22^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81189-1257.840 /\left(220.735+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -4.3 to $125.22^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
6570 (interpolated-Antoine eq., temp range $24.6-100.13^{\circ} \mathrm{C}$, Boublik et al. 1973, 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80304-1252.59 /\left(220.119+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ), temp range $24.6-100.13^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
6240 (interpolated-Antoine eq., temp range -36.5 to $99.2^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8548.0 /(\mathrm{T} / \mathrm{K})]+7.934852$; temp range -36.5 to $99.2^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{kPa})=5.92751-1252.348 /\left(220.09+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $69.2-271.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
6580 (interpolated-Antoine eq., temp range: $24-100^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81189-1257.84 /\left(220.74+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range: $24-100^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
6500 (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.92885-1153.36 /\left(220.241+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range not specified (Antoine eq., Riddick et al. 1986) 6580 (interpolated, Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93934-1254.146 /(-52.831+\mathrm{T} / \mathrm{K})$, temp range: 297-314 K, (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.44016-1650.17 /(\mathrm{T} / \mathrm{K})$; temp range $423-523 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.33252-1441.485 /(-36.695+\mathrm{T} / \mathrm{K})$; temp range $194-299 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.97534-1283 / 067 /(-40.166+\mathrm{T} / \mathrm{K})$; temp range $372-416 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.26002-1501.036 /(-19.15+\mathrm{T} / \mathrm{K})$; temp range $413-494 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.76427-3268.783 /(206.659+\mathrm{T} / \mathrm{K})$; temp range $490-544 \mathrm{~K}$ (Antoine eq.-VI, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=35.954-3.0569 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.8896 \cdot \log (\mathrm{~T} / \mathrm{K})-7.2916 \times 10^{-11} .(\mathrm{T} / \mathrm{K})+3.1060 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range 161-564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
308030 (calculated-P/C, Mackay \& Leinonen 1975)
330000; 308000, 365000 (recommended; calculated-P/C, Mackay \& Shiu 1981)
304960 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
472090, 110700 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
314110 (calculated-P/C, Lyman et al. 1982)
350140 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
327200 (calculated-P/C, Eastcott et al. 1988)
338270 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
5.83 (estimated-HPLC/MS, Burkhard et al. 1985)
4.54 (calculated-fragment const., Burkhard et al. 1985)
5.02 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
4.06 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization: volatilization $\mathrm{t}_{1 / 2}=5.5 \mathrm{~h}$ from a water column $1 \mathrm{~m}^{2}$ in cross section of depth 1 m (Mackay \& Leinonen 1975);
$\mathrm{t}_{1 / 2} \sim 3.1 \mathrm{~h}$ at $20^{\circ} \mathrm{C}$ in a river 1 m deep flowing at $1 \mathrm{~m} / \mathrm{s}$ with a wind velocity of $3 \mathrm{~m} / \mathrm{s}$ (estimated, Lyman et al. 1982).
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=2.83 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=2.35 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mole}^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range 298-493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{OH}}=3.73 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{O}(\mathrm{PP})}=9.10 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=3.7 \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule $^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{0} 3}{ }^{*}=2.0 \times 10^{-23} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range 298-323 K (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=(3.66 \pm 0.16) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=3.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K and $3.56 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=3.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=7.5 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=1.65 \times 10^{-16} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=3.57 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=9.0 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric lifetime was estimated to be 16 h , based on the photooxidation reaction rate constant of $3.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with OH radical in air during summer daylight (Altshuller 1991).
Surface water: volatilization $\mathrm{t}_{1 / 2}=5.5 \mathrm{~h}$ from a water column $1 \mathrm{~m}^{2}$ in cross section of depth $1-\mathrm{m}$ (Mackay \& Leinonen 1975);
estimated $\mathrm{t}_{1 / 2}=3.1 \mathrm{~h}$ at $20^{\circ} \mathrm{C}$ in a river 1 m deep flowing at $1 \mathrm{~m} / \mathrm{s}$ with a wind velocity of $3 \mathrm{~m} \mathrm{~s}^{-1}$ (Lyman et al. 1982).

### 2.1.1.1.15

2,3,4-Trimethylpentane


Common Name: 2,3,4-Trimethylpentane
Synonym:
Chemical Name: 2,3,4-trimethylpentane
CAS Registry No: 565-75-3
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{18} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{3}$
Molecular Weight: 114.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-109.2 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
113.5 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.7191 \quad$ (Weast 1984)
$0.7191,0.7191 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
158.9 (calculated-density, Stephenson \& Malanowski 1987) 185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $38.0,32.67\left(25^{\circ} \mathrm{C}\right.$, at normal bp, Dreisbach 1959)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 9.27 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 56.65, 38.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
2.34, $2.30 \quad\left(0 ; 25^{\circ} \mathrm{C}\right.$, shake flask-GC, Polak \& Lu 1973)
1.36 (shake flask-GC, Price 1976)
2.30, 1.36 (quoted lit., IUPAC Solubility Data Series, Shaw 1989)
2.86, 2.03 ( $0,25^{\circ} \mathrm{C}$, calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.85396-1315.034 /\left(217.526+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $36.568-114.381^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
3431 (Antoine eq. regression, temp range -26 to $113.5^{\circ} \mathrm{C}$ Stull 1947)
3600 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85396-1315.084 /\left(217.526+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $25-150^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
3600 (interpolated-Antoine eq., temp range $7.1-140.0^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85396-1315.084 /\left(217.526+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $7.1-140.0^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
3430 (interpolated-Antoine eq., temp range -26.3 to $113.5^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8988.2 /(\mathrm{T} / \mathrm{K})]+7.997094$; temp range -26.3 to $113.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$1179\left(4.912^{\circ} \mathrm{C}\right.$, static method-inclined piston manometer, measured range -50.325 to $4.912^{\circ} \mathrm{C}$, Osborn \& Douslin 1974)
3600 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.98137-1316.608 /\left(217.70+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $69.2-271.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
3600 (extrapolated-Antoine eq., temp range $36-114^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85396-1315.08 /\left(217.53+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $36-114^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
3610 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.00347-1330.047 /(-53.921+\mathrm{T} / \mathrm{K})$; temp range $288-400 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.37038-1511.86 /(-38.054+\mathrm{T} / \mathrm{K})$; temp range $223-289 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=35.1565-3.0232 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.2267 \cdot \log (\mathrm{~T} / \mathrm{K})+2.7691 \times 10^{-11} .(\mathrm{T} / \mathrm{K})+2.7828 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $164-566 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
190000; 302000, 179000 (recommended; calculated-P/C, Mackay \& Shiu 1981)
178700 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=6.99 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K , measured range $243-313 \mathrm{~K}$ (relative rate method with reference to $n$-hexane, Harris \& Kerr 1988; Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=7.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=7.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K and the atmospheric lifetime was estimated to be 20 h during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=7.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric lifetime was estimated to be 20 h , based on the photooxidation reaction rate constant of $7.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with OH radicals in air during summer daylight (Altshuller 1991).

### 2.1.1.1.16 <br> n-Hexane



Common Name: $n$-Hexane
Synonym: hexane
Chemical Name: $n$-hexane
CAS Registry No: 110-54-3
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{14} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{4} \mathrm{CH}_{3}$
Molecular Weight: 86.175
Melting Point ( $\left.{ }^{\circ} \mathrm{C}\right)$ : -95.35 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 68.73 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6593,0.6548 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 130.7; $131.6\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 31.552, $28.853 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986) 31.52 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 13.028 (Dreisbach 1959) 13.079 (Riddick et al. 1986) 13.08 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 73.22, 72.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$140 \quad\left(15.5^{\circ} \mathrm{C}\right.$, shake flask-cloud point, Fühner 1924)
$<262$ (shake flask-residue volume, Booth \& Everson 1948)
36.0 (shake flask-cloud point, Durand 1948)

120 (shake flask-cloud point, McBain \& Lissant 1951)
9.50 (shake flask-GC, McAuliffe 1963, 1966;)
16.2 (vapor saturation-GC, Barone et al. 1966)
18.3* (shake flask-GC, measured range $4-55^{\circ} \mathrm{C}$, Nelson \& De Ligny 1968)
12.3 (shake flask-GC, Leinonen \& Mackay 1973)
12.4* (shake flask-GC, Polak \& Lu 1973)
13.0 (shake flask-GC, Krasnoshchekova \& Gubertritis 1973)
16.2 (shake flask-GC, Mackay et al. 1975)
9.47* (shake flask-GC, measured range $25-151.8^{\circ} \mathrm{C}$, Price 1976)
12.3 (shake flask-GC, Aquan-Yuen et al. 1979)
10.09* (vapor saturation-GC, measured range $15.5-40^{\circ} \mathrm{C}$, Jönsson et al. 1982)
12.24 (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982; Miller et al. 1985)
14.1 (calculated-activity coeff. $\gamma$ and $\mathrm{K}_{\mathrm{ow}}$, Tewari et al. 1982b)
$11.4^{*} \quad\left(37.78^{\circ} \mathrm{C}\right.$, shake flask-GC, measured $37.78-200^{\circ} \mathrm{C}$, Tsonopoulos \& Wilson 1983)
9.55 (shake flask-GC, Coates et al. 1985)
14.0 (shake flask-purge and trap-GC, Coutant \& Keigley 1988)
9.8* (recommended best value, IUPAC Solubility Data Series, temp range $0-140^{\circ} \mathrm{C}$, Shaw 1989)
$\ln x=-374.90804+16327.128 /(\mathrm{T} / \mathrm{K})+53.89582 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)
11.5* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-425 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$24811^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, static-manometer, measured range $30-60^{\circ} \mathrm{C}$, Smyth \& Engel 1929)
$19920^{*} \quad\left(24.7^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $13.033-69.541^{\circ} \mathrm{C}$ Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87776-1171.530 /\left(224.366+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.033-69.541^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)
19700* (calculated-Antoine eq. regression, temp range -53.9 to $68.7^{\circ} \mathrm{C}$, Stull 1947)
20170 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87776-1171.53 /\left(224.366+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -10 to $110^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
20198* (interpolated-Antoine eq., temp range -25.1 to $92.1^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87776-1171.530 /\left(224.366+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -25.1 to $92.1^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
3120*
$\left(-0.51^{\circ} \mathrm{C}\right.$, gas saturation, measured range -95.44 to $-0.51^{\circ} \mathrm{C}$, Carruth \& Kobayashi 1973)
20130 (Campbell et al. 1968)
20124, 20141 (static method-differential pressure gauge, Bissell \& Williamson 1975)
22090* $\quad\left(27.1^{\circ} \mathrm{C}\right.$, Letcher \& Marsicano 1974)
21809, 57929,130189 ( $26.85,51.85,76.85^{\circ} \mathrm{C}$, vapor-liquid equilibrium VLE data, Gutsche \& Knapp 1982)
20160 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.01098-1176.102 /\left(224.899+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.033-69.54{ }^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.72763-1031.938 /\left(208.304+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $27.11-45.11^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Letcher \& Marsicano 1974, Boublik et al. 1984)
20190 (interpolated-Antoine eq., temp range -25 to $92^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87601-1171.17 /\left(224.41+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -25 to $92^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 20700, 20180, 20160(headspace-GC, correlated, Antoine eq., Hussam \& Carr 1985)
20170 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.00091-1171.91 /\left(224.408+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range not specified (Antoine eq., Riddick et al. 1986) 20180, 20300, 20165 (interpolated-Antoine equations I, II and IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.00431-1172.04 /(-48.747+\mathrm{T} / \mathrm{K})$; temp range $293-343 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.15142-1224.492 /(-45.358+\mathrm{T} / \mathrm{K})$; temp range $238-298 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.47892-1800.89 /(-4.115+\mathrm{T} / \mathrm{K})$; temp range $189-259 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99521-1167.388 /(-49.272+\mathrm{T} / \mathrm{K})$; temp range $298-341 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.91942-1123.687 /(-54.776+\mathrm{T} / \mathrm{K})$; temp range $341-377 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.4106-1469.286 /(-7.702+\mathrm{T} / \mathrm{K})$; temp range $374-451 \mathrm{~K}$ (Antoine eq.-VI, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.30814-2367.155 /(111.016+\mathrm{T} / \mathrm{K})$; temp range $445-508 \mathrm{~K}$ (Antoine eq.-VII, Stephenson \& Malanowski 1987)
10854 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)
20136* $\quad\left(24.96^{\circ} \mathrm{C}\right.$, Hg manometer, measured range $9.95-49.97^{\circ} \mathrm{C}$, Gracia et al. 1992)
20180* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{2.79797-2.022083 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+2.287564 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\} ;$ reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=341.863 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=69.7378-3.6278 \times 10^{3} /(\mathrm{T} / \mathrm{K})-23.927 \cdot \log (\mathrm{~T} / \mathrm{K})+1.281 \times 10^{-2} .(\mathrm{T} / \mathrm{K})-1.6844 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $178-507 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
24938, $53982\left(30,50^{\circ} \mathrm{C}\right.$, VLE equilibrium data, Carmona et al. 2000)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
183690
(calculated-1/K $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)

160000, 50590
190000
177060
173340*
(calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
(calculated-P/C, Mackay \& Shiu 1975,1981; Bobra et al. 1979)
(equilibrium cell-concn ratio-GC, Vejrosta et al. 1982)
(equilibrium cell-concentration ratio-GC, measured range $14.52-34.9^{\circ} \mathrm{C}$ Jönsson et al. 1982)
$103262,135400,172140,215420,261420\left(15,20,25,30,35^{\circ} \mathrm{C}\right.$, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=21493.1 /(\mathrm{T} / \mathrm{K})+59.299 \cdot \ln (\mathrm{~T} / \mathrm{K})-414.193$; temp range $15-35^{\circ} \mathrm{C}$ (least-square regression of equilibrium cell-conen ratio-GC measurements, Jönsson et al. 1982)
77820* (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm}_{-} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=25.25-7530 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
130790 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
18600* $\left(40^{\circ} \mathrm{C}\right.$, equilibrium headspace-GC, measured range $40-70^{\circ} \mathrm{C}$, Kolb et al. 1992)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=-28.60+8375 /(\mathrm{T} / \mathrm{K})$; temp range $40-70^{\circ} \mathrm{C}$ (equilibrium headspace-GC measurements, Kolb et al. 1992)

163812 (EPICS-GC, Ryu \& Park 1999)
$65318 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=12.150-3143 /(\mathrm{T} / \mathrm{K}) \quad$ (summary of literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {Ow }}$ :
3.00 (calculated- $\pi$ constant, Hansch et al. 1968; Hansch \& Leo 1979)
3.90 (shake flask-concn. ratio-GC, Platford 1979; Platford 1983)
4.20 (calculated-activity coeff. $\gamma$, Wasik et al. 1981, 1982)
4.11 (generator column-GC, Tewari et al. 1982a,b)
2.90 (HPLC-k' correlation, Coates et al. 1985)

425 (calculated-activity coeff., Berti et al. 1986)
4.16 (generator column-GC, Schantz \& Martire 1987)
4.00 (recommended, Sangster 1989, 1993)
4.29 (calculated-activity coeff., Tse \& Sandler 1994)
3.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.55* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range $20.29-50.28^{\circ} \mathrm{C}$ Gruber et al. 1997)
2.44 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=9.30 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atoms (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=(3.8 \pm 0.8) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 305 K (relative rate method, Llyod et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=5.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}}=(6.1-6.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} 292-303 \mathrm{~K}, \mathrm{k}_{\mathrm{OH}}($ calc $)=6.96 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 300 K (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=5.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=9.3 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atoms, at room temp. (abstraction mechanism, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=(5.71 \pm 0.09) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a)
$\mathrm{k}_{\mathrm{NO} 3}=(1.05 \pm 0.2) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984a, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=(5.70 \pm 0.09) \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=5.21 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=6.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=5.61 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991, Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=5.58 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.05 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{OH}}=5.61 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=10.5 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3}=1.05 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (Atkinson 1991)
$\mathrm{k}_{\mathrm{NO} 3}(\operatorname{exptl})=1.06 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}(\mathrm{calc})=1.11 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}} *=5.45 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=11 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=5.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $230-400 \mathrm{~K}$ (relative rate method, DeMore \& Bayes 1999)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction $\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ in air, based on reaction rate constant of $3.8 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with hydroxyl radical (Darnall et al. 1976);
atmospheric lifetime $\sim 25 \mathrm{~h}$, based on a rate constant of $5.61 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with OH radicals in summer daylight (Altshuller 1991).

## TABLE 2.1.1.1.16.1

Reported aqueous solubilities of $\boldsymbol{n}$-hexane at various temperatures
1.

| Nelson \& De Ligny 1968 |  | Polak \& Lu 1973 |  | Price 1976 |  | Jönsson et al. 1982 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-GC |  | shake flask-GC |  | vapor saturation-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 4.0 | 16.4 | 0 | 16.5 | 25.0 | 9.47 | 15 | 10.72 |
| 14.0 | 15.2 | 25 | 12.4 | 40.1 | 10.1 | 20 | 10.32 |
| 25.0 | 18.3 |  |  | 55.7 | 13.2 | 25 | 10.09 |
| 35.0 | 12.9 |  |  | 69.7 | 15.4 | 30 | 10.02 |
| 45.0 | 22.2 |  |  | 69.7 | 15.2 | 35 | 10.10 |
| 55.0 | 21.2 |  |  | 99.1 | 22.4 |  |  |
|  |  |  |  | 114.4 | 29.2 |  |  |
|  |  |  |  | 121.3 | 37.6 |  |  |
|  |  |  |  | 137.3 | 56.9 |  |  |
|  |  |  |  | 151.8 | 106.0 |  |  |

(Continued)

TABLE 2.1.1.1.16.1 (Continued)
2.

| Tsonopoulos \& Wilson 1983 |  | Shaw 1989a |  | Mạczyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | IUPAC recommended |  | calc-recommended LLE |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 37.78 | 11.4 | 0 | 17 | 0 | 15.8 |
| 93.33 | 27.4 | 20 | 12 | 4 | 14.36 |
| 94.4 | 25.6 | 24 | 11 | 13 | 12.45 |
| 100 | 29.7 | 30 | 9.9 | 15 | 12.45 |
| 148.09 | 130 | 40 | 11 | 20 | 12.0 |
| 150 | 162 | 50 | 12 | 25 | 11.5 |
| 200 | 885 | 60 | 13.6 | 30 | 11.5 |
|  |  | 70 | 15.7 | 35 | 11.5 |
|  |  | 80 | 18.5 | 40.1 | 11.5 |
|  |  | 100 | 27 | 55.7 | 12.93 |
|  |  | 120 | 45 | 69.7 | 15.32 |
|  |  | 140 | 80 | 99.1 | 26.33 |
|  |  |  |  | 113.8 | 37.34 |
|  |  |  |  | 121.3 | 44.52 |
|  |  |  |  | 137.2 | 67.02 |
|  |  |  |  | 151.8 | 105.3 |



FIGURE 2.1.1.1.16.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $n$-hexane.

TABLE 2.1.1.1.16.2
Reported vapor pressures of $n$-hexane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\{(\mathrm{T} / \mathrm{K})-\mathrm{C}\}$
(3a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{0} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{\mathrm{A}_{0}-\mathrm{A}_{1} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{A}_{2} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$
(5) - Cox eq.
1.

| Smyth \& Engel 1929 |  | Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static-manometer |  | ebulliometry |  | summary of literature data |  | selected values |  |
| $t^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |
| 30 | 24811 | 13.033 | 11698 | -53.9 | 133.3 | -25.19 | 1333 |
| 40 | 36757 | 16.576 | 13819 | -34.5 | 666.6 | -14.36 | 2666 |
| 50 | 53409 | 20.618 | 16620 | -25.0 | 1333 | -7.50 | 4000 |
| 60 | 75727 | 24.717 | 19920 | -14.1 | 2666 | -2.36 | 5333 |
|  |  | 28.528 | 23451 | -2.30 | 5333 | 1.79 | 6666 |
| bp/ ${ }^{\circ} \mathrm{C}$ | 68.8 | 33.631 | 28956 | 5.40 | 7999 | 5.31 | 7999 |
|  |  | 38.311 | 34896 | 15.8 | 13332 | 11.08 | 10666 |
|  |  | 43.967 | 43322 | 31.6 | 26664 | 15.762 | 13332 |
|  |  | 49.803 | 53655 | 49.8 | 53329 | 24.764 | 19998 |
|  |  | 56.030 | 66757 | 68.7 | 101325 | 31.572 | 26664 |
|  |  | 62.785 | 83719 |  |  | 37.114 | 33331 |
|  |  | 67.554 | 97605 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -95.3 | 41.824 | 39997 |
|  |  | 68.067 | 99201 |  |  | 49.612 | 53329 |
|  |  | 68.540 | 100694 |  |  | 55.973 | 66661 |
|  |  | 69.081 | 102394 |  |  | 61.394 | 79993 |
|  |  | 69.541 | 103913 |  |  | $66.145$ | $93326$ |
|  |  |  |  |  |  | $67.030$ | $95992$ |
|  |  | bp/ $/{ }^{\circ} \mathrm{C}$ | 68.740 |  |  | 67.896 | 98659 |
|  |  |  |  |  |  | 68.744 | 101325 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |
|  |  | A | 6.87776 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | B | 1171.530 |  |  | A | 6.87024 |
|  |  | C | 224.366 |  |  | B | 118.72 |
|  |  | temp ran | $3-69.5{ }^{\circ} \mathrm{C}$ |  |  | C | 224.210 |
|  |  |  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 68.744 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ} \mathrm{m}$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 31.55 |
|  |  |  |  |  |  | at bp | 28.85 |

(Continued)

TABLE 2.1.1.1.16.2 (Continued)
2.

| Carruth \& Kobayashi 1973 |  | Letcher \& Marsicano 1974 |  | Gracia et al. 1992 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation |  | static method-manometer |  | Hg manometer |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| -95.44 | 1.360 | 27.11 | 22091 | 9.95 | 10081 | 162.54 | 0.1 |
| -95.13 | 1.373 | 29.31 | 24151 | 14.98 | 12818 | 176.70 | 1.0 |
| -91.70 | 2.266 | 33.81 | 29197 | 19.97 | 16136 | 193.88 | 10 |
| -88.93 | 3.213 | 36.44 | 32437 | 24.96 | 20136 | 215.51 | 100 |
| -83.99 | 5.973 | 39.88 | 37117 | 29.96 | 24949 | 243.81 | 1000 |
| -75.94 | 13.60 | 42.45 | 40996 | 34.95 | 30577 | 282.95 | 10000 |
| -61.25 | 64.13 | 45.15 | 45289 | 39.93 | 37185 | 341.863 | 101325 |
| -53.29 | 128 | 48.11 | 50476 | 44.96 | 45000 | 298.15 | 20180 |
| -34.84 | 656 |  |  | 49.97 | 54028 |  |  |
| -24.91 | 1264 | Antoine eq |  |  |  | data cal | from Cox eq. |
| -14.39 | 2560 | eq. 3 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 5 | $\mathrm{P} / \mathrm{kPa}$ |
| -0.51 | 3120 | A | 6.6298 | Antoine eq. |  | $\mathrm{A}_{0}$ | 2.73425 |
|  |  | B | 1050.38 | eq. 3 a | $\mathrm{P} / \mathrm{kPa}$ | $\mathrm{A}_{1}$ | $2.02283 \times 10^{-3}$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -95.36 | C | 210.477 | A | 13.74029 | $\mathrm{A}_{2}$ | $2.287564 \times 10^{-6}$ |
|  |  |  |  | B | 2654.670 | with re | ence state at |
| eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=30.84$ |  | C | 50.869 | $\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}$ | 101.325 |
| A | 19.5553 |  |  |  |  | $\mathrm{T}_{0} / \mathrm{K}$ | 341.863 |
| B | 4292.8 |  |  |  |  |  |  |



FIGURE 2.1.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-hexane.

TABLE 2.1.1.1.16.3
Reported Henry's law constants and octanol-air partition coefficients of $n$-hexane at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

| Henry's law constant |  |  |  |  |  | $\log \mathrm{K}_{\mathrm{OA}}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Jönsson et al. 1982 |  | Ashworth et al. 1988 |  | Kolb et al. 1992 |  | Gruber et al. 1997 |  |
| equilibrium cell-GC |  | EPICS-GC |  | equilibrium headspace-GC |  | GC det'd activity coefficient |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\log \mathrm{K}_{\text {OA }}$ |
| 14.52 | 103536 | 10 | 24115 | 40 | 18600 | 20.29 | 2.548 |
| 14.52 | 103090 | 15 | 41847 | 60 | 64410 | 30.3 | 2.386 |
| 15.0 | 103262 | 20 | 89470 | 70 | 237750 | 40.4 | 2.216 |
| 20.05 | 135426 | 25 | 77818 |  |  | 50.28 | 2.090 |
| 20.05 | 136182 | 30 | 158067 | eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ |  |  |
| 20.0 | 135403 |  |  | A | -28.60 |  |  |
| 25 | 174565 | eq. 4 | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ | B | -8375 |  |  |
| 25 | 172140 | A | 25.25 |  |  |  |  |
| 25 | 172140 | B | 7530 |  |  |  |  |
| 30.2 | 215560 |  |  |  |  |  |  |
| 30.2 | 211937 |  |  |  |  |  |  |
| 30.0 | 215418 |  |  |  |  |  |  |
| 34.9 | 264034 |  |  |  |  |  |  |
| 34.9 | 256113 |  |  |  |  |  |  |
| 35.0 | 261424 |  |  |  |  |  |  |



FIGURE 2.1.1.1.16.3 Logarithm of Henry's law constant versus reciprocal temperature for $n$-hexane.


FIGURE 2.1.1.1.16.4 Logarithm of $K_{O A}$ versus reciprocal temperature for $n$-hexane.

### 2.1.1.1.17 <br> 2-Methylhexane (Isoheptane)



Common Name: 2-Methylhexane
Synonym: isoheptane, ethylisobutylmethane
Chemical Name: 2-methylhexane
CAS Registry No: 591-76-4
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{2}\left(\mathrm{CH}_{2}\right)_{2} \mathrm{CH}_{3}$
Molecular Weight: 100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-118.2 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 90.04 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6786,0.6744 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959) $0.6786,0.6548 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 147.66, $148.58 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 34.807, $30.669 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.184 (Dreisbach 1959; Riddick et al. 1986)
9.18 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
59.29, 57.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
2.54 (shake flask-GC, Price 1976)
3.51 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
8380 (calculated-Antoine eq. regression, temp range -40.4 to $90^{\circ} \mathrm{C}$, Stull 1947)
$9000 \quad\left(25.518^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $18.5-90.9^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87319-1236.026 /\left(219.545+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
8780 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87318-1236.026 /\left(219.545+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10-110^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
8780 (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=5.87318-1236.026 /\left(219.545+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -9.10 to $114.78^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
8370 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8538.7 /(\mathrm{T} / \mathrm{K})]+8.055523$; temp range -40.4 to $90^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 87778,8785 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.0031-1238.614 /\left(219.867+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $18.5-90.9^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.06712-1270.535 /\left(222.971+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-45^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
8790 (interpolated-Antoine eq., temp range -9 to $115^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87318-1236.026 /\left(219.55+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -9 to $115^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$

8800 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.99612-1235.10 /\left(219.469+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
8790 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.00513-1240.11 /(-53.123+\mathrm{T} / \mathrm{K})$; temp range $296-365 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=54.1075-3.785 \times 10^{3} /(\mathrm{T} / \mathrm{K})-17.547 \cdot \log (\mathrm{~T} / \mathrm{K})+8.2594 \times 10^{-3} .(\mathrm{T} / \mathrm{K})-3.4967 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $155-530 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):

```
346000 (calculated-P/C, Mackay & Shiu 1981, Eastcott et al. 1988)
346500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
51878* (26.9}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , EPICS-GC, measured range 26.9-45 ' C, Hansen et al. 1993)
ln}[\textrm{H}/(\textrm{kPa}\cdot\mp@subsup{\textrm{m}}{}{3}/\textrm{mol})]=3608/(\textrm{T}/\textrm{K})-8.0; temp range 26.9-45*'C (EPICS-GC, Hansen et al. 1993)
63856 (20 C C, selected from reported experimental determined values, Staudinger & Roberts 2001)
log K}\mp@subsup{\textrm{AW}}{\textrm{AW}}{}=-4.274+1669/(T/K)(summary of literature data, Staudinger & Roberts 2001
```


## Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=6.80 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson 1990, 1991)
$\mathrm{k}_{\mathrm{OH}}=6.80 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with atmospheric lifetime of 25 h in summer daylight (Altshuller 1990)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $6.80 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radicals and an estimated lifetime of 25 h in summer daylight (Altshuller 1990).

TABLE 2.1.1.1.17.1
Reported Henry's law constants of 2-methylhexane at various temperatures

| Hansen et al. $\mathbf{1 9 9 3}$ |  |
| :--- | :---: |
| EPICS-GC |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{k P a ~ m}{ }^{3} / \mathrm{mol}\right)$ |
| 26.9 | 51.878 |
| 35.0 | 31.512 |
| 45.0 | 25.939 |
| $\ln [\mathrm{H} /(\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol})]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| eq. 4 | $\mathrm{H} /(\mathrm{kPa} \mathrm{m} 3 / \mathrm{mol})$ |
| A | $-8 \pm 3.53$ |
| B | $-3608 \pm 1088$ |

### 2.1.1.1.18 <br> 3-Methylhexane



Common Name: 3-Methylhexane
Synonym: ethylmethylpropylmethane
Chemical Name: 3-methylhexane
CAS Registry No: 589-34-4
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16} ; \mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right)\left(\mathrm{CH}_{2}\right)_{2} \mathrm{CH}_{3}$
Molecular Weight: 100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-119.4 (Riddick et al. 1986; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
92 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.6860 \quad$ (Weast 1984)
$0.6871,0.6830 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
145.83, 146.71 (calculated-density)
162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 35.087, $30.79\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):

| 4.95 | (shake flask-GC, Polak \& Lu 1973) |
| :--- | :--- |
| 2.64 | (shake flask-GC, Price 1976) |
| 3.80 | (suggested IUPAC tentative value, Shaw 1989) |
| $6.12,4.29$ | $\left(0.25^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004) |

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
7782 (Antoine eq. regression, temp range -39 to $91.9^{\circ} \mathrm{C}$ Stull 1947)
$7702 \quad\left(23.662^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $19.915-92.737^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86754-1240.196 /\left(219.223+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $19.9-92.7^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
8210 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86764-1240.196 /\left(219.223+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10-130^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
8213 (interpolated-Antoine eq., temp range -7.90 to $116.73^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86764-1240.196 /\left(219.223+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -7.90 to $116.73^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
7772 (interpolated-Antoine eq., temp range -39.0 to $91.9^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8596.3 /(\mathrm{T} / \mathrm{K})]+8.065472$; temp range -39.0 to $91.9^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
8212 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.99489-1241.528 /\left(219.375+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-92.74^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
8210 (interpolated-Antoine eq., temp range -8 to $117^{\circ} \mathrm{C}$ Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86764-1240.196 /\left(219.22+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -8 to $117^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
8300 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.98993-1238.88 /\left(219.10+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
8215 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.9926-1239.57 /(-53.979+\mathrm{T} / \mathrm{K})$; temp range $289-366 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=35.2535-2.931 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.667 \cdot \log (\mathrm{~T} / \mathrm{K})-5.2026 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.2107 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $154-535 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
172000 (recommended, Mackay \& Shiu 1981)
312170 (calculated-P/C, Eastcott et al. 1988)
311620 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=7.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990,1991)
$\mathrm{k}_{\mathrm{OH}}=7.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ with a calculated atmospheric lifetime of 20 h during summer daylight (Altshuller 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
photooxidation reaction rate constant of $7.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical and an estimated lifetime of 20 h during summer daylight (Altshuller 1991).

### 2.1.1.1.19 <br> 2,2,5-Trimethylhexane



Common Name: 2,2,5-Trimethylhexane
Synonym:
Chemical Name: 2,2,5-trimethylhexane
CAS Registry No: 3522-94-9
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{20},\left(\mathrm{CH}_{3}\right)_{3} \mathrm{CCH}_{2} \mathrm{CH}_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 128.255
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-105.7 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 124.09 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $25^{\circ} \mathrm{C}$ ): $0.7072 \quad$ (Weast 1984) $0.7072,0.7032 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 181.3, $182.4 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 40.175, $33.76\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 6.192 (Riddick et al. 1986)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
1.15 (shake flask-GC, McAuliffe 1966)
$0.79 ; 0.54,0.54 \quad\left(0 ; 25^{\circ} \mathrm{C}\right.$, shake flask-GC, calculated-group contribution, Polak \& Lu 1973)
$0.80,0.80 \quad\left(0,25^{\circ} \mathrm{C}\right.$, IUPAC recommended best value, Shaw1989b)
0.613 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.83532-1324.049 /\left(210.737+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $46.1-125.0^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
2212 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83531-1324.059 /\left(210.737+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35-145^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
2210 (interpolated-Antoine eq., temp range $16.17-151.1^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83531-1324.049 /\left(210.737 \mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $16.17-151.1^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
2216 (static method-inclined piston manometer, measured range -35 to $30^{\circ} \mathrm{C}$, Osborn \& Douslin 1964)
2207 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.96385-1326.27 /\left(212.991+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $46.14-126.05^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
2207 (extrapolated-Antoine eq., temp range 46 to $125^{\circ} \mathrm{C}$ Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83775-1325.54 /\left(210.91+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $46-125^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
2216 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.96021-1324.049 /\left(210.737+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
2218 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.99253-1243.85 /(-60.158+\mathrm{T} / \mathrm{K})$; temp range $288-399 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.25179-1471.621 /(-48.901+\mathrm{T} / \mathrm{K})$; temp range $238-293 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=7.8816-2.6422 \times 10^{3} /(\mathrm{T} / \mathrm{K})+23.902 \cdot \log (\mathrm{~T} / \mathrm{K})-1.5376 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+7.7931 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $167-568 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
350000 (recommended, Mackay \& Shiu 1981)
523760 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.63 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
4.46 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants and Half-Lives:

Half-Lives in the Environment:

### 2.1.1.1.20 n-Heptane



Common Name: $n$-Heptane
Synonym: heptane
Chemical Name: $n$-heptane
CAS Registry No: 142-82-5
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{16}, \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{5} \mathrm{CH}_{3}$
Molecular Weight:100.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -90.55 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
98.4 (Dreisbach 1959; Weast 1972-73; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.6837 (Weast 1972-73)
0.6837, $0.6795 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
146.6, $147.5\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$36.55,31.7\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)
36.57 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
14.037 (Riddick et al. 1986)
14.04 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
76.9, 81.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$50.0 \quad\left(15.5^{\circ} \mathrm{C}\right.$, shake flask-cloud point, Fühner 1924)
150 (radiotracer method, Black et al. 1948)
$15.0 \quad\left(16^{\circ} \mathrm{C}\right.$, shake flask-cloud point, Durand 1948)
2.93 (shake flask-GC, McAuliffe 1963,1966)
11.0* $\quad\left(22^{\circ} \mathrm{C}\right.$, cloud point, measured range $295-355 \mathrm{~K}$ at $17-55 \mathrm{MPa}$, Connolly 1966)
2.66* (shake flask-GC, measured range $4.3-45^{\circ} \mathrm{C}$, Nelson \& De Ligny 1968)
4.39; 3.37* ( $0,25^{\circ} \mathrm{C}$, shake flask-GC, Polak \& Lu 1973)
2.57 (shake flask-GC, Krasnoshchekova \& Gubertritis 1975)
2.24* (shake flask-GC, measured range $25-150.4^{\circ} \mathrm{C}$, Price 1976)
3.70 (shake flask-GC, Bittrich et al. 1979)
2.90 (partition coefficient-GC, Rudakov \& Lutsyk 1979)
3.58 (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)
4.62 (calculated-activity coeff. $\gamma$ and $\mathrm{K}_{\mathrm{ow}}$, Tewari et al. 1982b)
2.51* (vapor saturation-GC, measured range $15-40^{\circ} \mathrm{C}$, Jönsson et al. 1982)
2.95 (shake flask-GC, Coates et al. 1985)
3.57 (lit. average, Riddick et al. 1986)
2.90 (shake flask-purge and trap-GC, Coutant \& Keigley 1988)
2.40* (recommended best value, IUPAC Solubility Data Series, temp range 0-140 ${ }^{\circ} \mathrm{C}$, Shaw 1989)
$\ln x=-396.93979+17232.298 /(\mathrm{T} / \mathrm{K})+56.95927 \cdot \ln (\mathrm{~T} / \mathrm{K})$, temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)
2.95* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-423.6 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
5520* $\quad\left(22.7^{\circ} \mathrm{C}\right.$, static-manometer, measured range $22.7-98.4^{\circ} \mathrm{C}$, Smyth \& Engel 1929)
$6370^{*} \quad\left(25.9^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $25.9-99.3^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90342-1268.636 /\left(216.951+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25.9-99.3^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
5795* (calculated-Antoine eq. regression, temp range -34 to $98.4^{\circ} \mathrm{C}$ Stull 1947)
6425* $\quad\left(26.039^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $26-99.3^{\circ} \mathrm{C}$ Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90027-1296.871 /\left(216.757+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $26.0-99.3^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
6110 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90240-1268.115 /\left(216.90+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15-155^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
6105 (Harris \& Dunlop 1970)
6113* (interpolated-Antoine eq., temp range -2.10 to $123.41^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90240-1268.115 /\left(216.900+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -2.10 to $123.41^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8409.6 /(\mathrm{T} / \mathrm{K})]+7.786586$; temp range -34.0 to $247.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
5080* ( $22.46^{\circ} \mathrm{C}$, gas saturation, measured range -87.85 to $22.46^{\circ} \mathrm{C}$, Carruth \& Kobayashi 1973)
6037, 6057 (static method-differential pressure gauge, Bissell \& Williamson 1975)
$7826,18929,40469,57059\left(30,50,70,80^{\circ} \mathrm{C}\right.$, vapor-liquid equilibrium VLE data, Gutsche \& Knapp 1982)
6090 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.02701-1167.592 /\left(216.796+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25.92-99.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=4.38001-668.768 /\left(159.522+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -87.85 to $22.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Carruth \& Kobayashi 1973, Boublik et al. 1984)
6110, 5958, 6090 (headspace-GC, correlated, Antoine eq., Hussam \& Carr 1985)
6090 (interpolated-Antoine eq., temp range -2 to $124^{\circ} \mathrm{C}$ Dean 1985. 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98677-1264.90 /\left(216.54+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -2 to $124^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
6090 (literature average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.02167-1264.90 /\left(216.544+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
6110 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.02633-1268.583 /(-56.054+\mathrm{T} / \mathrm{K})$; temp range 297-375 K (Antoine eq., Stephenson \& Malanowski 1987)
6102* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{2.86470-2.113204 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+2.250991 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=371.552 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=65.0257-3.8188 \times 10^{3} /(\mathrm{T} / \mathrm{K})-21.684 \cdot \log (\mathrm{~T} / \mathrm{K})+1.0387 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+1.0206 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $183-540 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$12309\left(40^{\circ} \mathrm{C}\right.$, average value, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)
$7811,18869\left(30,50^{\circ} \mathrm{C}\right.$, VLE equilibrium data, Carmona et al. 2000)
62503* (355.899 K, ebulliometry, measured range 355.899-503.406 K, Weber 2000)
Henry's Law Constant $\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right.$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

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206200 (calculated-1/K}\mp@subsup{\textrm{K}}{\textrm{AW}}{},\mp@subsup{\textrm{C}}{\textrm{W}}{}/\mp@subsup{\textrm{C}}{\textrm{A}}{},\mathrm{ , reported as exptl., Hine & Mookerjee 1975)
226000, 73120 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
230000 (recommended, Mackay & Shiu 1981)
250420* (25.04 ' C, equilibrium cell-concentration ratio-GC, measured range 15.3-35.05 ' C Jönsson
    et al. 1982)
136120, 184640, 243020, \(315050,394150\left(15,20,25,30,35^{\circ} \mathrm{C}\right.\), calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
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$\ln 1 / \mathrm{K}_{\mathrm{AW}}=23748.4 /(\mathrm{T} / \mathrm{K})+64.927 \cdot \ln (\mathrm{~T} / \mathrm{K})-454.172$; temp range $15-35^{\circ} \mathrm{C}$ (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)
273400 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
91294* ( $26^{\circ} \mathrm{C}$, EPICS-GC, measured range $26-45^{\circ} \mathrm{C}$, Hansen et al. 1993)
$\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-3730 /(\mathrm{T} / \mathrm{K})+17.0$; temp range $26-45^{\circ} \mathrm{C}$ (EPICS-GC, Hansen et al. 1993)
220825 (EPICS-GC, Ryu \& Park 1999)
$68000 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=6.532-1491 /(\mathrm{T} / \mathrm{K})$ (summary of literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
3.50 (calculated- $\pi$ constant, Hansch et al. 1968, Hansch \& Leo 1979)
4.76 (calculated-activity coeff. $\gamma$, Wasik et al. 1981,1982)
4.66 (generator column-GC, Tewari et al. 1982a,b)
3.44 (HPLC-k' correlation, Coates et al. 1985)
4.48 (Berti et al. 1986)
4.66, 4.72 (generator column-GC, calculated-activity coeff. $\gamma$, Schantz \& Martire 1987)
$4.50 \pm 0.25$ (recommended, Sangster 1989)
4.66 (recommended, Sangster 1993)
4.99 (calculated-activity coefficients, Tse \& Sandler 1994)
4.66 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
3.05* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\circ}$ in octanol, measured range 20.29-50.28 ${ }^{\circ} \mathrm{C}$ Gruber et al. 1997) 2.95 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=(7.30 \pm 0.17) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a, 1984c)
$\mathrm{k}_{\mathrm{NO} 3}=1.36 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1988,1990 )
$\mathrm{k}_{\mathrm{OH}}=7.52 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=7.15 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991)
$\mathrm{k}_{\mathrm{OH}}=7.15 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=1.36 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=7.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.36 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{OH}}=7.15 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K , with a calculated atmospheric lifetime of 19 h during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}=(1.34-1.37) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=(1.36,1.38) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ recommended $)=1.37 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}($ calc $)=1.45 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}} *=7.02 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=15 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:

Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $7.15 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radicals with an estimated lifetime of 19 h in summer daylight (Altshuller 1991).

TABLE 2.1.1.1.20.1
Reported aqueous solubilities of $\boldsymbol{n}$-heptane at various temperatures
1.

| Connolly 1966 |  | Nelson \& De Ligny 1968 |  | Polak \& Lu 1973 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-cloud point |  | shake flask-GC |  | shake flask-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 22 | 1.1 | 4.3 | 1.95 | 0 | 4.39 |
| 57 | 3.3 | 13.5 | 2.02 | 25 | 3.37 |
| 77 | 3.7 | 25.0 | 2.66 |  |  |
| 82 | 10.3 | 35.0 | 2.27 |  |  |

2. 

| Price 1976 |  | Jonsson et al. 1982 |  | Shaw 1989a |  | Mączyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | vapor saturation-GC |  | IUPAC "tentative" best values |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 25.0 | 2.24 | 15 | 2.67 | 0 | 3.0 | 0 | 4.18 |
| 40.1 | 2.63 | 20 | 2.57 | 10 | 2.0 | 15 | 3.23 |
| 55.7 | 3.11 | 25 | 2.51 | 20 | 2.4 | 20 | 3.06 |
| 99.1 | 5.60 | 30 | 2.49 | 25 | 2.4 | 25 | 2.95 |
| 118.0 | 11.4 | 35 | 2.52 | 30 | 2.40 | 30 | 2.90 |
| 136.6 | 27.3 |  |  | 40 | 2.5 | 35 | 2.90 |
| 150.4 | 43.7 |  |  | 50 | 2.9 | 40.1 | 2.95 |
|  |  |  |  | 60 | 3.3 | 45 | 3.01 |
|  |  |  |  | 90 | 3.9 | 55.7 | 3.34 |
|  |  |  |  | 100 | 5.8 | 99.1 | 7.79 |
|  |  |  |  | $120$ | 13 | 118 | 12.8 |
|  |  |  |  | 140 | 31 | 136.6 | 22.8 |
|  |  |  |  |  |  | 150.4 | 36.7 |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=-2.43$ |  |  |  |



FIGURE 2.1.1.1.20.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $n$-heptane.

TABLE 2.1.1.1.20.2
Reported vapor pressures of $n$-heptane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{\mathrm{A}_{0}-\mathrm{A}_{1} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{A}_{2} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$
(5) - Cox eq.
1.

| Smyth \& Engel 1929 |  | Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static method-manometer |  | ebulliometry |  | summary of literature data |  | ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 22.7 | 5520 | 25.925 | 6370 | -34.0 | 133.3 | 26.030 | 6425 |
| 30.0 | 7759 | 29.699 | 7665 | -12.7 | 666.6 | 29.813 | 7717 |
| 30.3 | 7839 | 33.024 | 8977 | -2.1 | 1333 | 33.108 | 9013 |
| 38.4 | 11466 | 36.017 | 10311 | 9.5 | 2666 | 36.105 | 10352 |
| 50.0 | 18812 | 38.822 | 11700 | 22.3 | 5333 | 38.901 | 11740 |
| 51.2 | 19998 | 42.599 | 13821 | 30.6 | 7999 | 42.680 | 13866 |
| 61.2 | 29331 | 46.929 | 16604 | 41.8 | 13332 | 46.987 | 16659 |
| 69.5 | 39703 | 51.320 | 19920 | 58.7 | 26664 | 51.373 | 19966 |
| 70.0 | 40183 | 55.394 | 23443 | 78.0 | 53329 | 55.442 | 23499 |
| 79.5 | 55955 | 60.862 | 28950 | 98.4 | 101325 | 60.902 | 29003 |
| 98.4 | 101325 | 65.882 | 34897 |  |  | 65.916 | 34948 |
|  |  | 71.930 | 43326 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -90.6 | 71.966 | 43386 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -90.5 | 78.160 | 53647 |  |  | 78.202 | 53270 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 98.4 | 84.823 | 66749 |  |  | 84.856 | 66815 |
|  |  | 92.053 | 83706 |  |  | 92.678 | 83769 |
|  |  | 97.154 | 97590 |  |  | 97.180 | 97663 |
|  |  | 97.702 | 99186 |  |  | 97.728 | 99257 |
|  |  | 98.207 | 100689 |  |  | 98.237 | 100758 |

(Continued)

## TABLE 2.1.1.1.20.2 (Continued)


2.

| Zwolins |  | Carruth \& Kobayashi 1973 |  | Ruzicka \& Majer 1994 |  | Weber 2000 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| selected values |  | gas saturation |  | recommended |  | ebulliometry |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | T/K | P/Pa |
| -2.22 | 1333 | -87.85 | 0.288 | -40 | 76.3 | 355.899 | 62503 |
| 9.43 | 2666 | -80.41 | 0.867 | -20 | 393 | 359.210 | 69482 |
| 16.78 | 4000 | -68.21 | 4.240 | 0 | 1520 | 363.492 | 79475 |
| 22.29 | 5333 | -55.70 | 16.40 | 20 | 4730 | 367.925 | 89500 |
| 26.75 | 6666 | -42.11 | 57.46 | 25 | 6102 | 370.925 | 99446 |
| 30.519 | 7999 | -27.95 | 196 | 40 | 12300 | 374.219 | 109546 |
| 36.706 | 10666 | -14.0 | 595 | 60 | 28100 | 377.268 | 119434 |
| 41.723 | 13332 | 1.01 | 1667 | 80 | 57100 | 380.130 | 129452 |
| 51.366 | 19998 | 11.92 | 2986 | 100 | 106000 | 382.836 | 139321 |
| 58.656 | 26664 | 22.46 | 5080 |  |  | 386.617 | 154371 |
| 64.591 | 33331 |  |  | OR |  | 390.085 | 169321 |
| 69.632 | 39997 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -90.60 | T/K | P/Pa | 394.397 | 189252 |
| 77.966 | 53329 |  |  | 179.40 | 0.1 | 335.188 | 30303 |
| 84.772 | 66661 | eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ | 194.52 | 1.0 | 339.317 | 35308 |
| 90.571 | 79993 | A | 20.1590 | 212.98 | 10 | 342.996 | 40310 |
| 95.650 | 93326 | B | 4852.65 | 236.18 | 100 | 349.358 | 50269 |
| 96.597 | 95992 |  |  | 266.53 | 1000 | 352.183 | 55286 |
| 97.523 | 98659 |  |  | 308.48 | 10000 | 354.804 | 60285 |
| 98.429 | 101325 |  |  | 371.55 | 101325 | 357.252 | 65269 |
|  |  |  |  | 298.15 | 6102 | 359.559 | 70277 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  | 363.894 | 60452 |
| A | 6.89385 |  |  | data ca | om Cox eq. | 367.733 | 90423 |
| B | 1264.37 |  |  | eq. 5 | P/kPa | 371.255 | 100423 |
| C | 216.636 |  |  | $\mathrm{A}_{0}$ | 2.86470 | 374.510 | 110415 |
| bp/ ${ }^{\circ} \mathrm{C}$ | 98.429 |  |  | $\mathrm{A}_{1}$ | $2.113204 \times 10^{-3}$ | 377.544 | 120394 |
| $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  | $\mathrm{A}_{2}$ | $2.250991 \times 10^{-6}$ | 380.390 | 130382 |
| at $25^{\circ} \mathrm{C}$ | 36.55 |  |  | with r | nce state at | 383.069 | 140381 |
| at bp | 31.70 |  |  | $\mathrm{P}_{0} / \mathrm{kPa}$ | 101.325 | 386.826 | 155364 |
|  |  |  |  | To/K | 371.552 | 390.313 | 170377 |
|  |  |  |  |  |  | 394.609 | 190385 |
|  |  |  |  |  |  | to |  |
|  |  |  |  |  |  | 503.406 | 1597746 |



FIGURE 2.1.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-heptane.

TABLE 2.1.1.1.20.3
Reported Henry's law constants and octanol-air water partition coefficients of $n$-heptane at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / K_{\text {AW }}\right)=A-B /(T / K)$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

Henry's law constant

| Jönsson et al. 1982 |  | Hansen et al. 1993 |  | Gruber et al. 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| equilibrium cell-GC |  | EPICS-GC |  | GC det'd activity coefficient |  |
| $t^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | $\mathrm{t}^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | $t /{ }^{\circ} \mathrm{C}$ | $\log \mathrm{K}_{\text {OA }}$ |
| 15.0 | 136118* | 26.0 | 91294 | 20.29 | 3.047 |
| 15.3 | 140244 | 35.8 | 121083 | 30.3 | 2.839 |
| 15.3 | 136260 | 45.0 | 193024 | 40.4 | 2.654 |
| 20.0 | 184640* |  |  | 50.28 | 2.510 |
| 20.05 | 190443 | eq. 4 | $\mathrm{H} /\left(\mathrm{kPa} \mathrm{m}^{3} / \mathrm{mol}\right)$ |  |  |
| 20.05 | 187513 | A | $17 \pm 2.22$ |  |  |
| 25.0 | 243021* | B | $3730 \pm 686$ |  |  |
| 25.05 | 193690 |  |  |  |  |
| 25.05 | 190710 |  |  |  |  |
| 25.04 | 250419 |  |  |  |  |
| 29.8 | 302857 |  |  |  |  |
| 29.8 | 316821 |  |  |  |  |
| 30.0 | 315049* |  |  |  |  |
| 35.05 | 389419 |  |  |  |  |
| 34.83 | 405792 |  |  |  |  |
| 34.83 | 379903 |  |  |  |  |
| 35.0 | 394148* |  |  |  |  |

* interpolated data


FIGURE 2.1.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for $n$-heptane.


FIGURE 2.1.1.1.20.4 Logarithm of $K_{O A}$ versus reciprocal temperature for $n$-heptane.

### 2.1.1.1.21 <br> 2-Methylheptane



Common Name: 2-Methylheptane
Synonym:
Chemical Name: 2-methylheptane
CAS Registry No: 592-27-8
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{18} ; \mathrm{CH}_{3} \mathrm{CH}\left(\mathrm{CH}_{3}\right)\left(\mathrm{CH}_{2}\right)_{4} \mathrm{CH}_{3}$
Molecular Weight: 114.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -109.02 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 117.66 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.698 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$163.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987; Ruelle \& Kesselring 1997) 185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $39.68,33.60\left(25^{\circ} \mathrm{C}\right.$, normal bp, Dreisbach 1959)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 11.92 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 72.62, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.95, $4.55 \quad$ (quoted, calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992) 2.84; 5.94 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)
$0.95 ; 1.61,1.61$ (quoted exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle \&
Kesselring 1997)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.91737-1337.468 /\left(213.693+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $41.7-118.5^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
2620 (calculated-Antoine eq. regression, temp range -21 to $117.6^{\circ} \mathrm{C}$ Stull 1947)
$6386 \quad\left(23.4^{\circ} \mathrm{C}\right.$, Nicolini \& Laffitte 1949)
2748 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91735-1337.468 /\left(213.693+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35-150^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
2748 (interpolated-Antoine eq., temp range $12.3-143.8^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91735-1337.468 /\left(213.693+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $12.3-143.8^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
2620 (interpolated-Antoine eq., temp range $-21-117.6^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9362.0 /(\mathrm{T} / \mathrm{K})]+8.154424$; temp range $-21-117.6^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 2732, 6850 (calculated-Antoine eq., Boublik et al. 1973, 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88814-1319.539 /\left(211.625+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $41-118.5^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85999-1313.125 /\left(230.02+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $23.4-75^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Nicolini \& Laffitte 1949, Boublik et al. 1973)
$1161 \quad\left(10^{\circ} \mathrm{C}\right.$, static method-inclined piston manometer, measured range -40 to $10^{\circ} \mathrm{C}$, Osborn \& Douslin 1974)

2750
(extrapolated-Antoine eq., temp range $42-119^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91735-1337.47 /\left(213.69+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $42-119^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
2750 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.05858-1346.996 /(-30.648+\mathrm{T} / \mathrm{K})$; temp range $285-392 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.81199-1703.6 /(-30.648+\mathrm{T} / \mathrm{K})$; temp range $233-286 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=37.693-3.2611 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.391 \cdot \log (\mathrm{~T} / \mathrm{K})-1.0524 \times 10^{-12} .(\mathrm{T} / \mathrm{K})+3.056 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $164-560 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
369880 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.91 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
4.04 (calculated $-\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}($ calc $)=8.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (SAR structure reactivity relationship, Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}=8.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated atmospheric lifetime $\tau=17 \mathrm{~h}$ during summer daylight hours (Altshuller 1991).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $8.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical and an estimated lifetime of 17 h during summer daylight (Altshuller 1991).

### 2.1.1.1.22 <br> 3-Methylheptane



Common Name: 3-Methylheptane Synonym:
Chemical Name: 3-methylheptane
CAS Registry No: 589-81-1
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{18} ; \mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right)\left(\mathrm{CH}_{2}\right)_{3} \mathrm{CH}_{3}$
Molecular Weight: 114.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-120.48 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 118.9 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
0.7075 (Weast 1984)
$0.7058,0.7018 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $161.4\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987) 185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 39.83, $34.08 \quad\left(25^{\circ} \mathrm{C}\right.$, normal bp, Dreisbach 1959)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 11.38 (Dreisbach 1959) 11.7 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 76.6, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.792 (shake flask-GC, Price 1976; quoted, Mackay \& Shiu 1981; Shaw 1989; Myrdal et al. 1992)
0.850 (estimated-nomograph, Brookman et al. 1985)
1.015 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.89945-1331.530 /\left(212.414+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $42.7-119.8^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry, manometer, Willingham et al. 1945)
2610 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.89944-1331.530 /\left(212.414+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $30-150^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
2600 (interpolated-Antoine eq., temp range $13.3-145.2^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.89944-1331.530 /\left(212.414+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $13.3-145.2^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
2466 (interpolated-Antoine eq., temp range -19.8 to $118.9^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9432.0 /(\mathrm{T} / \mathrm{K})]+8.179407$; temp range -19.8 to $118.9^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$1486 \quad\left(15^{\circ} \mathrm{C}\right.$, static method-inclined piston manometer, measured range -35 to $15^{\circ} \mathrm{C}$, Osborn \& Douslin 1974)

2600, 3232 (quoted, calculated-bp, Mackay et al. 1982)
2600 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.01647-1326.329 /\left(211.776+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $42.67-119.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
2605 (extrapolated, Antoine eq., temp range 43-120 ${ }^{\circ} \mathrm{C}$ Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.89944-1331.53 /\left(212.41+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $43-120^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)

2630 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.02047-1329.42 /(-60.945+\mathrm{T} / \mathrm{K})$; temp range $286-393 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.50909-1567.45 /(-40.786+\mathrm{T} / \mathrm{K})$; temp range $238-286 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=52.8828-3.6231 \times 10^{3} /(\mathrm{T} / \mathrm{K})-16.804 \cdot \log (\mathrm{~T} / \mathrm{K})+7.1828 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+7.4077 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $153-564 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ ):
376000 (calculated-P/C, Mackay \& Shiu 1981)
375900 (selected, Mills et al. 1982)
375800 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}($ calc $)=8.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR, Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}=8.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated atmospheric lifetime $\tau=16 \mathrm{~h}$ during summer daylight hours (Altshuller 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $8.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical with an estimated lifetime of 16 h during summer daylight (Altshuller 1991).

### 2.1.1.1.23 n-Octane



Common Name: $n$-Octane
Synonym: octane
Chemical Name: $n$-octane
CAS Registry No: 111-65-9
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{18} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{6} \mathrm{CH}_{3}$
Molecular Weight: 114.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -56.82 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 125.67 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.7027,0.6886 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
$0.70256 \quad\left(20^{\circ} \mathrm{C}\right.$, digital precision densimeter, Dejoz et al. 1996)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
162.6, $165.8\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
185.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 41.49, $34.431 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)
$41.56 \quad$ (298.15 K, recommended, Ruzicka \& Majer 1994)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 20.74 (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 95.86, 91.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
14.0 (cloud point, Fühner 1924, quoted, Deno \& Berkheimer 1960)
0.66 (shake flask-GC, McAuliffe 1963, 1966)
0.493 (radiotracer method, Baker 1967)
0.880* (shake flask-GC, measured range $5-25^{\circ} \mathrm{C}$, Nelson \& De Ligny 1968)
0.700 (shake flask-GC, Krzsnoshchekova \& Gubergrits 1973)
1.35; $0.85 \quad\left(0,25^{\circ} \mathrm{C}\right.$, shake flask-GC, Polak \& Lu 1973)
$0.431^{*} \quad$ (shake flask-GC, measured range $25149.5^{\circ} \mathrm{C}$, Price 1976)
0.615* (vapor saturation-GC, measured range $15-35^{\circ} \mathrm{C}$, Jönsson et al. 1982)
1.103 (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)
1.56 (calculated-activity coeff. and $\mathrm{K}_{\mathrm{OW}}$, Tewari et al. 1982b)
0.615 (vapor saturation-partition coefficient-GC, Jönsson et al. 1982)
0.660 (shake flask-GC, Coates et al. 1985)
$0.762^{*} \quad\left(37.75^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $37.75-280^{\circ} \mathrm{C}$, pressure range $0.0103-8.86 \mathrm{MPa}$, Heidmen et al. 1985)
$\ln x=-343.1497+13862.49 /(\mathrm{T} / \mathrm{K})+49.24600 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $37.75-280^{\circ} \mathrm{C}$ (shake flask-GC, Heidman et al. 1985)
$0.884,0.949\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, Burris \& MacIntyre 1986)
1.250 (shake flask-purge and trap-GC, Coutant \& Keigley 1988)
$0.71^{*} \quad$ (recommended, temp range $0-100^{\circ} \mathrm{C}$, IUPAC Solubility Data Series, Shaw 1989)
$\ln x=-415.7563+17975.386 /(\mathrm{T} / \mathrm{K})+59.55451 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)
$0.774^{*} \quad\left(29.9^{\circ} \mathrm{C}\right.$, shake flask-solid extraction-GC/FID, measured range $29.9-183^{\circ} \mathrm{C}$, Marche et al. 2003) $\ln x=-362.618+14904.474 /(\mathrm{T} / \mathrm{K})+52.067 \cdot \ln (\mathrm{~T} / \mathrm{K})$ : temp range $29.9-183^{\circ} \mathrm{C}$ (shake flask-solid extractionGC/FID measurements, Marche et al. 2003)
0.635* (calculated-liquid-liquid equilibrium LLE data, temp range 288.2-36.1 K, Ma̧czyński et al. 2004)
$0.807 \quad\left(24.9^{\circ} \mathrm{C}\right.$, generator column-GC/FID, measured range $10-45^{\circ} \mathrm{C}$, Sarraute et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$486.6^{*} \quad\left(3.7^{\circ} \mathrm{C}\right.$, static-McLeod gauge, measured range -9.31 to $3.7^{\circ} \mathrm{C}$, Linder 1931)
$7670^{*} \quad\left(52.972^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $52.972-126.570^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92377-1355.126 /\left(209.517+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $52.9-126.6^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
$1777^{*} \quad$ (calculated-Antoine eq. regression, temp range -14 to $125.6^{\circ} \mathrm{C}$, Stull 1947)
1870 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92377-1355.126 /\left(209.517+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $40-155^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
1885* (interpolated-Antoine eq., temp range $19.2-152.1^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971
$\log (\mathrm{P} / \mathrm{mmHg})=6.92377-11355.126 /\left(209.517+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $19.2-152.1^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
1825 (interpolated-Antoine eq., temp range -14 to $281.4^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9221.0 /(\mathrm{T} / \mathrm{K})]+7.894018$; temp range -14 to $281.4^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$1573^{*} \quad\left(23.96^{\circ} \mathrm{C}\right.$, gas saturation, measured range -56.35 to $23.96^{\circ} \mathrm{C}$, Carruth \& Kobayashi 1973)
1885, 2060 (quoted, calculated-bp, Mackay et al. 1982)
1860 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.04394-1351.938 /\left(209.12+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $52.93-126.57^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
1860 (interpolated-Antoine eq., temp range $19-152^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91868-1351.99 /\left(209.15+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $19-152^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
1870 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.04358-1351.99 /\left(209.155+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 1854, 1814, 1854 (headspace-GC, correlated, Antoine eq., Hussam \& Carr 1985)
1862 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.04231-1351.491 /(-64.014+\mathrm{T} / \mathrm{K})$; temp range $297-400 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.90115-2238.9 /(-4.53+\mathrm{T} / \mathrm{K})$; temp range $216-278 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16936-1440.32 /(-52.894+\mathrm{T} / \mathrm{K})$; temp range $396-432 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.23406-1492.068 /(-45.851+\mathrm{T} / \mathrm{K})$; temp range $428-510 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.66614-7.66614 /(159.091+\mathrm{T} / \mathrm{K})$; temp range $506-569 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
1872* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{2.90150-2.046204 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+2.010759 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=398.793 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=29.0948-3.0114 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.2653 \cdot \log (\mathrm{~T} / \mathrm{K})-2.2696 \times 10^{-11} .(\mathrm{T} / \mathrm{K})+1.468 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $216-569 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
1820* $\quad\left(24.6^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $291.25-409.95 \mathrm{~K}$, Dejoz et al. 1996)
$\ln (\mathrm{P} / \mathrm{Pa})=13.9183-3114.43 /[(\mathrm{T} / \mathrm{K})-63.9225]$; temp range $291-409 \mathrm{~K}$ (ebulliometry, Dejoz et al. 1996)
$6727^{*} \quad\left(50.43^{\circ} \mathrm{C}\right.$, comparative ebulliometry, measured range $323-563 \mathrm{~K}$, data fitted to Wagner eq., Ewing \& Ochoa 2003)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):

| 326800 | (calculated-1/K $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee) |
| :--- | :--- |
| 311900,110670 | (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 325300 | (calculated-P/C, Mackay \& Leinonen 1975; Mackay \& Shiu 1990) |
| 323200 | (calculated-P/C, Bobra et al. 1979; Mackay et al. 1979; Mackay 1981) |

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325000 (calculated-P/C, Mackay \& Shiu 1981)
355500* \(\left(25.1^{\circ} \mathrm{C}\right.\), equilibrium cell-concentration ratio-GC, measured range \(14.8-34.92^{\circ} \mathrm{C}\), Jönsson et al.
1982)
180130, \(253880,344280,458250,595800\left(15,20,25,30,35^{\circ} \mathrm{C}\right.\), calculated-temp dependence eq. derived from
exptl. data, Jönsson et al. 1982)
\(\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=26003.7 /(\mathrm{T} / \mathrm{K})+70.571 \cdot \ln (\mathrm{~T} / \mathrm{K})-494.151\); temp range: \(15-35^{\circ} \mathrm{C}\) (least-square regression of
    equilibrium cell-conen ratio-GC measurements, Jönsson et al. 1982)
324200 (calculated-P/C, Lyman et al. 1982)
\(\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{MPa}\right)=357.733-19363.1 /(\mathrm{T} / \mathrm{K})-9.04865 \cdot(\mathrm{~T} / \mathrm{K})^{2}-49.5296 \cdot \ln (\mathrm{~T} / \mathrm{K}) ;\) maximum \(\mathrm{k}_{\mathrm{H}}=7.836 \times 10^{4} \mathrm{MPa}\)
    at 372.1 K (Heidman et al. 1985)
314700 (calculated-P/C, Eastcott et al. 1988)
326200 (Valsaraj 1988)
201500 (calculated-MCI \(\chi\), Nirmalakhandan \& Speece 1988)
499500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
39213* \(\quad\left(27.9^{\circ} \mathrm{C}\right.\), EPICS-GC, measured range \(27.9-45^{\circ} \mathrm{C}\), Hansen et al. 1993)
\(\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-8014 /(\mathrm{T} / \mathrm{K})+30.0\); temp range: \(27.9-45^{\circ} \mathrm{C}(\) EPICS-GC, Hansen et al. 1993 \()\)
297951 (EPICS-GC, Ryu \& Park 1999)
\(21838\left(20^{\circ} \mathrm{C}\right.\), selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001)
\(\log \mathrm{K}_{\mathrm{AW}}=12.08-3263 /(\mathrm{T} / \mathrm{K})\) (summary of literature data, Staudinger \& Roberts 2001)
\(257797 \quad\left(24.9^{\circ} \mathrm{C}\right.\), calculated-P/C, Sarraute et al. 2004)
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
4.0 (calculated- \(\pi\) substituent const., Hansch et al. 1968; Hansch \& Leo 1979)
5.29 (calculated-activity coefficient \(\gamma\), Wasik et al. 1981,1982)
5.18 (generator column-GC, Tewari et al. 1982a,b)
4.0 (HPLC-k' correlation, Coates et al. 1985)
5.24 (generator column-GC, calculated-activity coefficient \(\gamma\), Schantz \& Martire 1987)
\(5.15 \pm 0.45\) (recommended, Sangster 1989; 1993)
5.61 (calculated-activity coefficients, Tse \& Sandler 1994)
5.18 (recommended, Hansch et al. 1995)
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Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section:
$3.55^{*} \quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\circ}$ in octanol, measured range $20.29-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997) 3.30 (calculated-measured $\gamma^{\circ}$ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $t_{1 / 2}=5.55 \mathrm{~h}$ for a water column of $1 \mathrm{~m}^{2}$ minimum cross section of depth 1 m (Mackay \& Leinonen 1975)
estimated $t_{1 / 2} \sim 3.1 \mathrm{~h}$ at $20^{\circ} \mathrm{C}$ in a river 1 m deep flowing at $1 \mathrm{~m} \mathrm{~s}^{-1}$ and with a wind velocity of $3 \mathrm{~m} \mathrm{~s}^{-1}$ (Lyman et al. 1982).
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=6.03 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ calc $)=2.35 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 296 K , measured range 296-497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.70 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}(\operatorname{exptl})=8.42 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \mathrm{~K}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=7.35 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 300 K (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=(9.01 \pm 0.19) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a, 1984c)
$\mathrm{k}_{\mathrm{OH}}=8.80 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=8.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=8.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=1.81 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=8.71 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.81 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{OH}}=8.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, estimated atmospheric lifetime of 16 h (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}=1.82 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=8.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Paulson \& Seinfeld 1992)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=1.84 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}($ calc $)=1.79 \times 10^{-16} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=8.71 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}^{*}=1.9 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for $\mathrm{C}_{4} \mathrm{H}_{10}$ and higher paraffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
photooxidation reaction $\mathrm{k}=8.68 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with OH radicals with an estimated lifetime of 16 h in air during summer daylight (Altshuller 1991).
Surface water: volatilization $t_{1 / 2}=5.55 \mathrm{~h}$ for a water column of $1 \mathrm{~m}^{2}$ minimum cross section of depth 1 m (Mackay
\& Leinonen 1975); estimated volatilization $\mathrm{t}_{1 / 2}=3.1 \mathrm{~h}$ at $20^{\circ} \mathrm{C}$ in a river 1 m deep flowing at $1 \mathrm{~m} / \mathrm{s}$ and with a wind velocity of $3 \mathrm{~m} / \mathrm{s}$ (Lyman et al. 1982).
Ground water:
Sediment:
Soil:
Biota:

TABLE 2.1.1.1.23.1
Reported aqueous solubilities of $\boldsymbol{n}$-octane at various temperatures
1.

| Nelson \& De Ligny 1968 |  | Polak \& Lu 1973 |  | Price 1976 |  | Jonsson et al. 1982 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-GC/FID |  | shake flask-GC |  | vapor saturation-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 5 | 1.65 | 0 | 1.35 | 25.0 | 0.431 | 15 | 0.653 |
| 15 | 0.89 | 25 | 0.85 | 40.1 | 0.524 | 20 | 0.628 |
| 25 | 1.84 |  |  | 69.7 | 0.907 | 25 | 0.615 |
|  |  |  |  | 99.1 | 1.12 | 30 | 0.612 |
|  |  |  |  | 121.3 | 4.62 | 35 | 0.620 |
|  |  |  |  | 136.6 | 8.52 |  |  |
|  |  |  |  | 149.5 | 11.80 |  |  |

TABLE 2.1.1.1.23.1 (Continued)
2.

| Heidman et al. 1985 | Shaw 1989a |  | Marche et al. 2003 |  | Mączy ${ }^{\text {chiski et al. } 2004}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC | IUPAC "tentative" best values |  | shake flask-GC |  | $\begin{aligned} & \text { calc-recommended LLE } \\ & \text { data } \end{aligned}$ |  |
| $\mathrm{t}^{\circ} \mathrm{C} \mathbf{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 37.75 | 0 | 0.14 | 29.9 | 0.774 | 15 | 0.698 |
| 93.35 | 20 | 0.63 | 30.3 | 0.762 | 20 | 0.698 |
| 148.85 | 25 | 0.71 | 69.2 | 1.517 | 25 | 0.635 |
| 206.35 25 | 30 | 0.61 | 70 | 2.234 | 30 | 0.635 |
| 262.35 220 | 40 | 0.8 | 99.9 | 3.046 | 35 | 0.635 |
| 279.65 380 | 50 | 1 | 101.1 | 3.414 | 37.7 | 0.635 |
|  | 60 | 1.2 | 124 | 7.806 | 40.1 | 0.952 |
| pressures range from 0.0103 to 8.86 MPa | 70 | 1.5 | 124 | 9.011 | 69.7 | 4.00 |
|  | 80 | 2 | 131 | 11.23 | 121.3 | 6.98 |
| $0.0103 \text { to } 8.86 \mathrm{MPa}$ | 90 | 2.7 | 131 | 12.25 | 136.6 | 12.06 |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=13.3$ | 100 | 3.7 | 151.2 | 24.88 | 149.5 | 22.21 |
| $25^{\circ} \mathrm{C}$ | 120 | 7.2 | 165.1 | 43.79 | 262.9 | 50.77 |
|  | 140 | 15 | 165.4 | 43.28 |  |  |
|  | 160 | 22 | 183 | 84.85 |  |  |
|  |  |  | $\ln x=\mathrm{A}+\mathrm{B} / \mathrm{T}+\mathrm{C} \cdot \ln \mathrm{T}$ |  |  |  |
|  |  |  |  | T in K |  |  |
|  |  |  | A | -362.618 |  |  |
|  |  |  | B | $14904.474$ |  |  |
|  |  |  | C | 52.067 |  |  |



FIGURE 2.1.1.1.23.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $n$-octane.

TABLE 2.1.1.1.23.2
Reported vapor pressures of $\boldsymbol{n}$-octane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$

$$
\begin{align*}
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1}\\
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)  \tag{2}\\
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})
\end{align*}
$$

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4)
(4a)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{\mathrm{A}_{0}-\mathrm{A}_{1} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{A}_{2} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$
(5) - Cox eq.
1.

| Linder 1931 |  | Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| McLeod gauge |  | ebulliometry |  | summary of literature data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -9.31 | 196.0 | 52.972 | 7670 | -14.0 | 133.3 | 19.03 | 1333 |
| -3.0 | 309.3 | 56.456 | 8979 | 8.30 | 666.6 | 39.06 | 2666 |
| 3.7 | 486.6 | 59.615 | 10314 | 10.2 | 1333 | 39.10 | 4000 |
|  |  | 62.592 | 11702 | 31.5 | 2666 | 44.95 | 5333 |
|  |  | 66.587 | 13823 | 45.1 | 5333 | 49.68 | 6666 |
|  |  | 71.163 | 16600 | 53.8 | 7999 | 53.67 | 7999 |
|  |  | 75.820 | 19918 | 65.7 | 13332 | 60.24 | 10666 |
|  |  | 80.134 | 23441 | 83.6 | 26664 | 65.56 | 13332 |
|  |  | 85.916 | $28952$ | 104.0 | 53329 | 75.79 | 19998 |
|  |  | 91.230 | $34894$ | 125.6 | 101325 | 83.52 | 26664 |
|  |  | 97.635 | 43326 |  |  | 89.813 | 33331 |
|  |  | 104.233 | 53646 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -56.8 | 95.158 | 39997 |
|  |  | 111.277 | 66742 |  |  | 103.991 | 53329 |
|  |  | $118.924$ | 83695 |  |  | 111.204 | 66661 |
|  |  | $124.319$ | 97584 |  |  | 117.349 | 79993 |
|  |  | 124.809 | 99161 |  |  | 122.731 | 93326 |
|  |  | 125.433 | 100662 |  |  | 123.734 | 95992 |
|  |  | 126.035 | 102386 |  |  | 124.715 | 98659 |
|  |  | 126.570 | 103900 |  |  | 125.675 | 101325 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 123.665 |  |  |  |  |
|  |  | $\text { eq. } 2$ | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | A | 6.92377 |  |  | A | 6.90940 |
|  |  | B | $1355.126$ |  |  | B | 1349.82 |
|  |  | C | 209.517 |  |  | C | 209.385 |
|  |  | temp ran | 9-126.6 ${ }^{\circ} \mathrm{C}$ |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 125.675 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{V}$ | $\mathrm{ol}^{-1}$ ) |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | $41.49$ |
|  |  |  |  |  |  | at bp | 34.41 |

TABLE 2.1.1.1.23.2 (Continued)
2.

| Carruth \& Kobayashi 1973 |  | Ruzicka \& Majer 1994 |  | Dejoz et al. 1996 |  | Ewing \& Ochoa 2003 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation |  | recommended |  | vapor-liquid equilibrium |  | comparative ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -56.35 | 2.40 | 194.67 | 0.1 | 18.1 | 1250 | 50.03 | 6727 |
| -54.64 | 2.746 | 210.84 | 1.0 | 20.7 | 1450 | 51.811 | 7640 |
| -49.92 | 4.40 | 230.53 | 10 | 24.69 | 1820 | 60.642 | 10766 |
| -42.73 | 9.706 | 255.25 | 100 | 27.4 | 2130 | 67.754 | 14507 |
| -35.08 | 20.13 | 287.52 | 1000 | 29.6 | 2410 | 73.195 | 18016 |
| -23.06 | 59.33 | 332.03 | 10000 | 31.2 | 2630 | 79.794 | 23174 |
| -13.75 | 127.7 | 398.79 | 101325 | 33.8 | 3020 | 88.950 | 32265 |
| 5.26 | 532.0 | 298.15 | 1872 | 36.8 | 3520 | 93.009 | 37123 |
| 16.41 | 1047 |  |  | 42.4 | 4670 | 99.293 | 45789 |
| 23.96 | 1573 | data calc. from Cox eq. eq. 5 <br> P/kPa |  | 48.6 | 6290 | 104.234 | 53686 |
|  |  |  |  | 51.4 | 7150 | 110.649 | 65523 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -56.81 | $\mathrm{A}_{0}$ | 2.90150 | 55.7 | 8690 | 115.266 | 75253 |
|  |  | $\mathrm{A}_{1}$ | $2.046204 \times 10^{-3}$ | 58.9 | 10000 | 118.867 | 83613 |
| eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ | $\mathrm{A}_{2}$ | $2.010759 \times 10^{-6}$ | 61.4 | 11130 | 121.958 | 91358 |
| A | $20.3621$ | with reference state at |  | 64.0 | 12410 | 125.705 | 101486 |
| B | 5294.36 | $\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}$ | 101.325 | 66.7 | 13890 | 128.458 | 109480 |
|  |  | $\mathrm{T}_{0} / \mathrm{K}$ | 398.793 | 68.3 | 14820 | 131.853 | 130296 |
|  |  |  |  | 71.8 | 17050 | 134.957 | 138.490 |
|  |  |  |  | 74.9 | 19240 |  |  |
|  |  |  |  | 77.6 | 21330 | Antoine eq. for $\mathrm{P}<145 \mathrm{kPa}$ in the following form $\ln \mathrm{P} / \mathrm{kPa}=(\mathrm{A}-\mathrm{B}) /(\mathrm{T}-\mathrm{C})$ with |  |
|  |  |  |  | 80.7 | 23900 |  |  |  |
|  |  |  |  | 85.3 | 28330 |  |  |  |
|  |  |  |  | 90.05 | 34030 |  |  |  |
|  |  |  |  | 96.1 | 41180 | A | 13.91204 |
|  |  |  |  | 100.5 | 47680 | B | 3110.704 |
|  |  |  |  | 102.2 | 50300 | C | 64.086 |
|  |  |  |  | eq. 3(a) | kPa | for tem | -563 K |
|  |  |  |  | A | 13.9183 | or pressur | $2301 \mathrm{kPa}$ |
|  |  |  |  | B | $3114.43$ | data fitted | agner eq. |
|  |  |  |  | C | -63.925 |  |  |
|  |  |  |  | for temp 29 |  |  |  |



FIGURE 2.1.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-octane.

TABLE 2.1.1.1.23.3
Reported Henry's law constants and octanol-air partition coefficients of $\boldsymbol{n}$-octane at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

Henry's law constant

| Jönsson et al. 1982 |  | Hansen et al. 1993 |  | Gru | al. 1997 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| equilibrium cell-GC |  | EPICS-GC |  | GC det'd activity coefficient |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} K_{\text {OA }}$ |
| 14.8 | 171001 | 27.9 | 39213 | 20.29 | 3.554 |
| 14.8 | 176031 | 35.0 | 93827 | 30.3 | 3.302 |
| 15.0 | 180126* | 45.0 | 167693 | 40.4 | 3.089 |
| 20.0 | 253880* |  |  | 50.28 | 2.927 |
| 20.05 | 259326 | eq. 4 | $\mathrm{H} /\left(\mathrm{kPa} \mathrm{m}^{3} / \mathrm{mol}\right)$ |  |  |
| 20.05 | 256596 | A | $30 \pm 5.25$ |  |  |
| 25.0 | 344280* | B | $8014 \pm 1617$ |  |  |
| 25.1 | 357298 |  |  |  |  |
| 25.1 | 353730 |  |  |  |  |
| 30.0 | 458253* |  |  |  |  |
| 30.1 | 452643 |  |  |  |  |
| 34.92 | 587452 |  |  |  |  |
| 35.0 | 595804* |  |  |  |  |
| * interpolated data |  |  |  |  |  |



FIGURE 2.1.1.1.23.3 Logarithm of Henry's law constant versus reciprocal temperature for $n$-octane.


FIGURE 2.1.1.1.23.4 Logarithm of $\mathrm{K}_{\mathrm{OA}}$ versus reciprocal temperature for $n$-octane.

### 2.1.1.1.24



Common Name: 4-Methyloctane
Synonym:
Chemical Name: 4-methyloctane
CAS Registry No: 2216-34-4
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{20} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right)\left(\mathrm{CH}_{2}\right)_{3} \mathrm{CH}_{3}$
Molecular Weight: 128.255
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-113.3 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
142.4 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.7199,0.7169 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$178.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$44.75,36.60\left(25^{\circ} \mathrm{C}\right.$, normal bp, Dreisbach 1961)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.115 (shake flask-GC, Price 1976; quoted, Shaw 1989)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
901 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9155-1406.0 /\left(206.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $50-165^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

933 (extrapolated-Antoine eq., temp range $32-170^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90318-1399.12 /\left(205.41+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32-170^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=11.2012-2.9467 \times 10^{3} /(\mathrm{T} / \mathrm{K})+1.2133 \cdot \log (\mathrm{~T} / \mathrm{K})-1.4423 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+9.177 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $160-588 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
1010000; 1000000 (calculated-P/C, recommended, Mackay \& Shiu 1981)
1007000 (selected, Mills et al. 1982)
1007000 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=9.72 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=9.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

### 2.1.1.1.25

n-Nonane


Common Name: $n$-Nonane
Synonym: nonane
Chemical Name: $n$-nonane
CAS Registry No: 111-84-2
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{20} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{7} \mathrm{CH}_{3}$
Molecular Weight: 128.255
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -53.46 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 150.82 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.7176,0.7138 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959) 0.7177, $0.7138 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 178.7, $179.7 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
44.442, $36.915 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)
$46.55 \quad$ (298.15 K, recommended, Ruzicka \& Majer 1994)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
15.468 (Dreisbach 1959; Riddick et al. 1986)
$6.28,15.38$ ( $-55.95,-53.45^{\circ} \mathrm{C}$, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
99.2, 100.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
0.220 (shake flask-GC, McAuliffe 1969;)
0.098 (Baker 1967)
0.071 (shake flask-GC, Krasnoshchekova \& Gubertritis 1973)
0.122* (shake flask-GC, measured range $25-136.6^{\circ} \mathrm{C}$, Price 1976)
$0.289,0.272\left(15,20^{\circ} \mathrm{C}\right.$, vapor saturation-GC, Jönsson et al. 1982)
0.219 (shake flask-GC, Coates et al. 1985)
1.70* (tentative best value, temp range $20-130^{\circ} \mathrm{C}$, IUPAC Solubility Data Series, Shaw 1989)
$\ln x=-433.434+18767.82 /(\mathrm{T} / \mathrm{K})+61.940 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from lit. calorimetric and solubility data, Tsonopoulos 1999)
0.135, $0.477 \quad\left(25,100.1^{\circ} \mathrm{C}\right.$, calculated-liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$6349^{*} \quad\left(70.127^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $70.127-151.764^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.94495-1435.158 /\left(202.331+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70.1-151.8^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
623* (calculated-Antoine eq. regression, temp range $1.4-149.5^{\circ} \mathrm{C}$, Stull 1947)
$6405^{*} \quad\left(70.343^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $70.343-151.786^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93513-1428.811 /\left(201.619+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70.343-151.786^{\circ} \mathrm{C}$ (Antoine eq., ebulliome-try-manometer measurements, Forziati et al. 1949)
580 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93513-1428.811 /\left(201.619+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $60-185^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
$571^{*} \quad$ (extrapolated-Antoine eq., temp range $39.32-178.48^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93513-1428.811 /\left(201.619+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $39.32-178.48^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10456.9 /(\mathrm{T} / \mathrm{K})]+8.332532$; temp range $2.4-149.5^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$404.0^{*} \quad\left(20.99^{\circ} \mathrm{C}\right.$, gas saturation, measured range -53.49 to $34.59^{\circ} \mathrm{C}$, Carruth \& Kobayashi 1973)
570, 713 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.0628-1430.638 /\left(201.827+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ), temp range: $70.434-151.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.0847-1439.2 /\left(205.962+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range: $66.61-147.86^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data Forziati et al. 1949, Boublik et al. 1984)
571 (extrapolated-Antoine eq., temp range $39-179^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93893-1431.82 /\left(202.01+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $39-179^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
570 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.06383-1431.82 /\left(202.011+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
517; 571 (extrapolated-Antoine eq.-I; interpolated-Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.0593-1429.46 /(-71.33+\mathrm{T} / \mathrm{K})$; temp range $344-426 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.17855-2523.8 /(\mathrm{T} / \mathrm{K})$; temp range $219-308 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987) 580.7* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{2.94690-2.061933 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.903683 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\} ;$ reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=423.932 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=8.8817-2.8042 \times 10^{3} /(\mathrm{T} / \mathrm{K})+1.5262 \cdot \log (\mathrm{~T} / \mathrm{K})-1.0464 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+5.7972 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $220-596 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
601000, 748000, 333000; 500000 (calculated-P/C values, recommended, Mackay \& Shiu 1981)
147400*, $372820\left(14.8,20.05^{\circ} \mathrm{C}\right.$, equilibrium cell-concentration ratio-GC, Jönsson et al. 1982)
173520, $348200 \quad\left(15,20^{\circ} \mathrm{C}\right.$, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=28259 /(\mathrm{T} / \mathrm{K})+76.183 \cdot \ln (\mathrm{~T} / \mathrm{K})-524.13$; temp range $15-35^{\circ} \mathrm{C}$ (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)
41950* (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \mathrm{m} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-0.1847+202.1 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
599600 (calculated-P/C, Eastcott et al. 1988)
601000 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
459668 (EPICS-GC, Ryu \& Park 1999)
$42164 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=1.104+39 /(\mathrm{T} / \mathrm{K})$ (summary of literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
4.51 (estimated-HPLC- $\mathrm{k}^{\prime}$ correlation, Coates et al. 1985)
$5.65 \pm 0.60$ (recommended, Sangster 1989)
5.42 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor,

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(10.7 \pm 0.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a, 1984c)
$\mathrm{k}_{\mathrm{OH}}=10.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=1.02 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=1.02 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=2.39 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=1.02 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ estimated atmospheric lifetime of 14 h (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=1.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=2.30 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=2.41 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (Atkinson 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=(1.92,2.59) \times 10^{-16} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=2.47 \times 10^{-16} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=10.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=2.3 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for $\mathrm{C}_{4} \mathrm{H}_{10}$ and higher paraffins for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); photooxidation reaction rate constant of $1.02 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with OH radical with an estimated lifetime $\tau=14 \mathrm{~h}$ during summer daylight (Altshuller 1991).

TABLE 2.1.1.1.25.1
Reported aqueous solubilities of $\boldsymbol{n}$-nonane at various temperatures

| Price 1976 |  | Jonsson et al. 1982 |  | Shaw 1989a |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | vapor saturation-GC |  | IUPAC "tentative" best |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 25.0 | 0.122 | 15 | 0.289 | 20 | 0.29 |
| 69.7 | 0.309 | 20 | 0.272 | 25 | 0.17 |
| 99.1 | 0.420 |  |  | 30 | 0.14 |
| 121.3 | 1.70 |  |  | 40 | 0.17 |
| 136.6 | 5.07 |  |  | 50 | 0.22 |
|  |  |  |  | 60 | 0.26 |
|  |  |  |  | 70 | 0.31 |
|  |  |  |  | 80 | 0.34 |
|  |  |  |  | 90 | 0.37 |
|  |  |  |  | 100 | 0.42 |
|  |  |  |  | 110 | 0.80 |
|  |  |  |  | 120 | 1.60 |
|  |  |  |  | 130 | 3.20 |



FIGURE 2.1.1.1.25.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $n$-nonane.

## TABLE 2.1.1.1.25.2

Reported vapor pressures of n-nonane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{0} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{0} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{\mathrm{A}_{0}-\mathrm{A}_{1} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{A}_{2} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$
(5) - Cox eq.
1.

| Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry-manometer |  | summary of literature data |  | ebulliometry-manometer |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 70.127 | 6349 | 2.4 | 133.3 | 70.343 | 6405 | 39.06 | 1333 |
| 74.388 | 7650 | 26.3 | 666.6 | 74.546 | 7697 | 51.93 | 2666 |
| 78.097 | 8955 | 38.0 | 1333 | 78.219 | 8995 | 60.12 | 4000 |
| 81.458 | 10294 | 51.0 | 2666 | 81.548 | 10335 | 66.25 | 5333 |
| 84.582 | 11687 | 65.6 | 5333 | 84.658 | 11724 | 71.216 | 6666 |
| 88.801 | 13822 | 74.1 | 7999 | 88.864 | 13847 | 75.409 | 7999 |
| 93.610 | 16611 | 86.0 | 13332 | 93.601 | 16639 | 82.293 | 10666 |
| 98.491 | 19913 | 104.7 | 26664 | 98.545 | 19949 | 87.873 | 13332 |
| 103.047 | 23451 | 126.8 | 53329 | 103.072 | 23479 | 98.593 | 19998 |
| 109.115 | 28952 | 149.5 | 101325 | 109.136 | 28984 | 106.694 | 26664 |
| 114.684 | 34892 |  |  | 114.712 | 34.930 | 113.284 | 33331 |
| 121.399 | 43319 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -53.7 | 121.433 | 43366 | 118.882 | 39997 |
| 128.329 | 53653 |  |  | 128.357 | 53703 | 128.131 | 53329 |
| 136.721 | 66757 |  |  | 135.741 | 66801 | 135.680 | 66661 |
| 143.738 | 83721 |  |  | 143.751 | 83755 | 142.110 | 79993 |
| 149.394 | 97609 |  |  | 149.409 | 97652 | 147.741 | 93326 |

(Continued)

| TABLE 2.1.1.1.25.2 (Continued) |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| ebulliometry-manometer |  | summary of literature data |  | ebulliometry-manometer |  | selected values |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
| 150.002 | 99207 |  |  | 150.017 | 99241 | 148.790 | 95992 |
| 150.565 | 100833 |  |  | 150.579 | 100734 | 149.816 | 98659 |
| 151.195 | 102401 |  |  | 151.222 | 102467 | 150.321 | 101325 |
| 151.764 | 103921 |  |  | 151.786 | 104006 |  |  |
|  |  |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| bp/ ${ }^{\circ} \mathrm{C}$ | 150.796 |  |  | bp/ $/{ }^{\circ} \mathrm{C}$ | 150.798 | A | 6.93440 |
|  |  |  |  |  |  | B | 1508.75 |
| eq. 2 | P/mmHg |  |  | eq. 2 | P/mmHg | C | 195.374 |
| A | 6.94445 |  |  | A | 6.93513 | bp/ ${ }^{\circ} \mathrm{C}$ | 150.821 |
| B | 1435.158 |  |  | B | 1428.811 |  | $\mathrm{mol}^{-1}$ ) |
| C | 202.331 |  |  | C | 201.619 | at $25^{\circ} \mathrm{C}$ | 36.92 |
| temp range: $70.1-151.8^{\circ} \mathrm{C}$ |  |  |  | temp rang | . $3-151.8^{\circ} \mathrm{C}$ | at bp | 46.44 |

2. 

Carruth \& Kobayashi 1973
Ruzicka \& Majer 1994
recommended

| gas saturation |  | recommended |  |
| :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathrm{P} / \mathrm{Pa}$ |
| -53.49 | 0.7586 | 209.23 | 0.1 |
| -49.4 | 0.825 | 226.30 | 1.0 |
| -48.26 | 0.925 | 247,08 | 10 |
| -36.32 | 3.240 | 273.13 | 100 |
| -27.45 | 7.866 | 307.09 | 1000 |
| -9.97 | 37.33 | 353.86 | 10000 |
| 2.60 | 100.4 | 423.392 | 101325 |
| 20.99 | 404.0 | 298.15 | 580.7 |
| 26.9 | 602.6 |  |  |
| 34.59 | 722.6 | data calc. from Cox eq. |  |
|  |  | eq. 5 | P/kPa |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -53.7 | $\mathrm{A}_{0}$ | 2.94690 |
|  |  | $\mathrm{A}_{1}$ | $2.051933 \times 10^{-3}$ |
| eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ | $\mathrm{A}_{2}$ | $1.903683 \times 10^{-6}$ |
| A | 20.8468 | with reference state at |  |
| B | -5811.26 | $\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}$ | 101.325 |
|  |  | $\mathrm{T}_{0} / \mathrm{K}$ | 423.392 |



FIGURE 2.1.1.1.25.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-nonane.

TABLE 2.1.1.1.25.3
Reported Henry's law constants of $\boldsymbol{n}$-nonane at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(5)
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

Jönsson et al. 1982
Ashworth et al. 1988

| equilibrium cell-GC |  | EPICS-GC |  |
| :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ |
| 14.8 | 244287 | 10 | 40530 |
| 14.8 | 221668 | 15 | 50257 |
| 15.0 | 237196 | 20 | 33640 |
| 20.0 | 348179 | 25 | 41949 |
| 20.05 | 369343 | 30 | 47116 |
| 20.05 | 363831 |  |  |
|  |  | eq. 4 a | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ |
|  |  | A | -0.1847 |
|  |  | B | 202.1 |



FIGURE 2.1.1.1.25.3 Logarithm of Henry's law constant versus reciprocal temperature for $n$-nonane.

### 2.1.1.1.26 <br> n-Decane



Common Name: $n$-Decane
Synonym: decane
Chemical Name: n-decane
CAS Registry No: 124-18-5
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{22} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{8} \mathrm{CH}_{3}$
Molecular Weight: 142.282
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-29.6 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 174.15 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7301,0.7273\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959) 0.7301, $0.7264\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 194.9, $195.9\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 229.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 51.367, $31.279\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986) 51.42 (209.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 28.72 (Dreisbach 1959)
28.677 (Riddick et al. 1986) 28.7 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : $117.99,109.8$ (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
0.016 (radiotracer, Baker 1958, 1959)
0.0198 (shake flask-GC, Franks 1966)
0.022 (Baker 1967)
0.052 (shake flask-GC, McAuliffe 1969)
0.0087 (shake flask-GC, Krasnoshchekova \& Gubertritis 1973)
$0.182,1.220$ (shake flask-headspace-GC, Mackay et al. 1975)
0.0029 (shake flask-refractometer, Becke \& Quitzsch 1977)
0.0524 (shake flask-GC, Coates et al. 1985)
$0.02,0.015\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, tentative best values, IUPAC Solubility Data Series, Shaw 1989)
$0.0277,0.0261\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, temp range 273.2-422.7 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$62.66^{*} \quad\left(8.50^{\circ} \mathrm{C}\right.$, static-McLeod gauge, measured range -3.80 to $8.50^{\circ} \mathrm{C}$, Linder 1931)
$7649^{*} \quad\left(94.481^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $94.481-175.121^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95367-1501.268 /\left(194.480+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $94.6-175.1^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
238* (calculated-Antoine eq. regression, temp range $17.1-173^{\circ} \mathrm{C}$, Stull 1947)
182 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95367-1501.268 /\left(194.480+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-210^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
180* (extrapolated-Antoine eq., temp range $57.7-202.9^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95367-1501.268 /\left(194.480+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $57.7-202.9^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10912.0 /(\mathrm{T} / \mathrm{K})]+8.248089$; temp range $17.1-173^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$86.53^{*} \quad\left(16.74^{\circ} \mathrm{C}\right.$, gas saturation, measured range -29.65 to $37.45^{\circ} \mathrm{C}$, Carruth \& Kobayashi 1973)
174 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.08321-1504.405 /\left(194.831+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $94.48-175.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
173 (extrapolated-Antoine eq., temp range $58-203^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.94365-1495.17 /\left(193.86+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $58-203^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$180^{*} \quad\left(24.941^{\circ} \mathrm{C}\right.$, gas saturation, measured temp range $298.091-347.887 \mathrm{~K}$, Allemand et al. 1986)
170 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.55216-1594.49 /\left(126.36+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
171 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.80914-1900.343 /(-47.319+\mathrm{T} / \mathrm{K})$; temp range $252-383 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.09206-1510.415 /(-77.646+\mathrm{T} / \mathrm{K})$; temp range $373-443 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.04899-1482.502 /(-80.635+\mathrm{T} / \mathrm{K})$; temp range $447-526 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=9.71412-6858.314 /(454.63+\mathrm{T} / \mathrm{K})$; temp range $524-617 \mathrm{~K}$ (Antoine eq.IV, Stephenson \& Malanowski 1987)
$874.1^{*} \quad\left(50.64^{\circ} \mathrm{C}\right.$, static-quartz pressure gauge, measured range $50.64-314.982^{\circ} \mathrm{C}$, Morgan \& Kobayashi 1994)

182* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{2.96690-1.932579 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+1.644626 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=447.269 \mathrm{~K}($ Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=26.5125-3.3584 \times 10^{3} /(\mathrm{T} / \mathrm{K})-6.1174 \cdot \log (\mathrm{~T} / \mathrm{K})-3.3225 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+4.8554 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $243-618 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$127.6^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, ebulliometer and inclined piston gauge, measured temp range $268-490 \mathrm{~K}$. Chirico et al. 1989)
324 (liquid $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation; Donovan 1996)
520* (41.6 ${ }^{\circ} \mathrm{C}$, ebulliometry, measured range $314.75-458.45 \mathrm{~K}$, Dejoz et al. 1996)
$\ln (\mathrm{P} / \mathrm{kPa})=13.9735-3441.40 /[(\mathrm{T} / \mathrm{K})-79.434]$; temp range $314.75-458.45 \mathrm{~K}$ (ebulliometry, Dejoz et al. 1996)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 326300 | (calculated-P/C, Mackay \& Shiu 1975) |
| :--- | :--- |
| 499500 | (calculated-P/C, Bobra et al. 1979; Mackay et al. 1979; selected, Mills et al. 1982) |
| 489400 | (calculated-P/C, Mackay 1981) |
| $700000 ;$ | 500000,108000 (recommended; calculated-P/C, Mackay \& Shiu 1981) |
| 431100 | (calculated-P/C, Eastcott et al. 1988) |
| 477870 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
5.67 (estimated-fragment const., Lyman 1982)
6.69, 5.98 (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)
5.01 (estimated, Coates et al. 1985)
$6.25 \pm 0.70$ (recommended, Sangster 1989)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :

Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(11.4 \pm 0.6) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $299 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982a, 1984c)
$\mathrm{k}_{\mathrm{OH}}=11.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=1.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)
$\mathrm{k}_{\mathrm{OH}}=11.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , atmospheric lifetime of 12 h during summer daylight (Altshuller 1991)
$\mathrm{k}_{\mathrm{NO} 3}(\operatorname{exptl})=2.59 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}(\mathrm{calc})=2.47 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm \mathrm{K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}} *=11.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=2.8 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24$ h for $\mathrm{C}_{4} \mathrm{H}_{10}$ and higher paraffins for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
photooxidation reaction rate constant $\mathrm{k}=1.16 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical with an estimated lifetime of 12 h during summer daylight (Altshuller 1991).

## TABLE 2.1.1.1.26.1

Reported vapor pressures of $n$-decane at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{array}{lll}
\log P=A-B /(T / K) & (1) & \ln P=A-B /(T / K) \\
\log P=A-B /\left(C+t /{ }^{\circ} C\right) & (2) & \ln P=A-B /\left(C+t /{ }^{\circ} C\right) \\
\log P=A-B /(C+T / K) & (3) & \ln P=A-B /(C+T / K) \\
\log P=A-B /(T / K)-C \cdot \log (T / K) & (4) & \\
\ln \left(P / P_{\text {ref }}\right)=\left[1-\left(T_{\text {ref }} / T\right)\right] \cdot \exp \left(a+b T+\mathrm{cT}^{2}\right) & (5) &
\end{array}
$$

1. 

| Linder 1931 |  | Willingham et al. 1945 |  | Stull 1947 |  | $\underline{\text { Zwolinski \& Wilhoit } 1971}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static-McLeod gauge |  | ebulliometry |  | summary of literature data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -3.80 | 22.0 | 94.481 | 7649 | 17.1 | 133.3 | 57.6 | 1333 |
| 0.20 | 28.0 | 98.352 | 8954 | 42.5 | 666.6 | 71.06 | 2666 |
| 0.50 | 30.66 | 101.859 | 10292 | 55.4 | 1333 | 79.61 | 4000 |
| 8.50 | 62.66 | 105.118 | 11686 | 69.1 | 2666 | 86.02 | 5333 |
|  |  | 109.526 | 13812 | 84.6 | 5333 | 91.20 | 6666 |
|  |  | 114.540 | 16609 | 94.6 | 7999 | 95.576 | 7999 |
|  |  | 119.640 | 19913 | 108.0 | 13332 | 102.759 | 10666 |
|  |  | 124.372 | 23451 | 127.8 | 26664 | 108.579 | 13332 |
|  |  | 130.690 | 28951 | 149.9 | 53329 | 119.759 | 19998 |
|  |  | 136.490 | 34892 | 173.0 | 101325 | 128.203 | 26664 |

(Continued)

TABLE 2.1.1.1.26.1 (Continued)

2.

## Carruth \& Kobayashi 1973

Allemand et al. 1986
Chirico et al. 1989

| gas saturation |  | gas saturation |  | ebulliometry |  | inclined piston gauge |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -29.65 | 1.72 | 24.941 | 180.0 | 100.086 | 9596 | -5.002 | 17.0 |
| -21.84 | 3.20 | 30.022 | 253.3 | 103.317 | 10897 | -0.002 | 26.4 |
| -18.68 | 4.586 | 35.019 | 352.0 | 106.561 | 12348 | 9.994 | 59.9 |
| -9.54 | 10.60 | 40.005 | 481.3 | 109.82 | 13961 | 19.999 | 127.6 |
| 4.35 | 33.20 | 45.002 | 650.6 | 113.09 | 15752 | 30.001 | 256.1 |
| 16.74 | 86.53 | 50.006 | 874.6 | 116.373 | 17737 | 34.999 | 355.0 |
| 31.45 | 186.7 | 55.001 | 1161 | 119.67 | 19933 | 40.0 | 486.3 |
| 37.45 | 205.3 | 59.996 | 1520 | 126.299 | 25023 | 44.0 | 657.8 |
|  |  | 64.916 | 1969 | 132.983 | 31177 | 50.0 | 879.9 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -29.71 | 70.049 | 2545 | 139.716 | 39565 | 60.006 | 1523.8 |
|  |  | 74.737 | 3190 | 146.502 | 47375 | 80.002 | 2536.1 |
| eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ |  |  | 153.399 | 57817 | 75.001 | 3227.1 |
| A | 20.8865 |  |  | 160.227 | 70120 |  |  |
| B | 6170.32 |  |  | 167.167 | 84533 |  |  |
|  |  |  |  | 174.157 | 101325 | Cox eq. |  |
|  |  |  |  | 181.199 | 120790 | eq. 5a | $\mathrm{P} / \mathrm{kPa}$ |
|  |  |  |  | 188.291 | 143250 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
|  |  |  |  | 195.43 | 169920 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 447.307 |
|  |  |  |  | 202.622 | 198490 | a | 2.96081 |
|  |  |  |  | 209.859 | 232020 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -1.90111 |
|  |  |  |  | 217.142 | 270020 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.60359 |
|  |  |  |  |  |  | temp rang | 68-490 K |

TABLE 2.1.1.1.26.1 (Continued)
3.

| Morgan \& Kobayashi 1994 |  | Ruzicka \& Majer 1994 |  | Dejoz et al. 1996 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static-quartz pressure gauge |  | recommended |  | vapor-liquid equilibrium |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa |
| 50.64 | 874.1 | 222.67 | 0.1 | 41.6 | 520 | 144.1 | 44090 |
| 59.933 | 1509 | 240.65 | 1.0 | 45.2 | 650 | 146.7 | 47640 |
| 79.938 | 4050 | 262.50 | 10 | 49.5 | 840 | 149.3 | 51420 |
| 99.970 | 9562 | 289.84 | 100 | 55.2 | 1170 | 151.2 | 54380 |
| 119.981 | 20150 | 325.64 | 1000 | 60.1 | 1520 | 153.4 | 57920 |
| 119.971 | 20154 | 374.25 | 10000 | 69.1 | 2410 | 156.5 | 63220 |
| 139.972 | 38892 | 447.27 | 101325 | 75.8 | 3330 | 159.3 | 69330 |
| 159.973 | 69695 | 298.15 | 182.0 | 84.2 | 4900 | 162.3 | 74190 |
| 179.974 | 117250 |  |  | 93.1 | 7200 | 165.5 | 80890 |
| 199.976 | 187250 | Cox eq. |  | 97.9 | 8760 | 168.4 | 87350 |
| 219.976 | 285770 | eq. 5 | P/kPa | 100.7 | 9820 | 174.6 | 102460 |
| 239.979 | . 420380 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 | 103.5 | 10970 | 178.9 | 114160 |
| 259.979 | 598790 | $\mathrm{Tref}_{\text {re }} / \mathrm{K}$ | 447.27 | 105.9 | 12020 | 182.7 | 125370 |
| 279.98 | 830150 | a | 2.96690 | 108.3 | 13180 | 185.3 | 133470 |
| 299.98 | 1125900 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -1.932579 | 110. | 14250 |  |  |
| 314.982 | 1395000 | $10^{6} / \mathrm{K}^{-2}$ | 1.644626 | 113.3 | 15870 | eq. 3(a) | P/kPa |
|  |  |  |  | 117.1 | 18200 | A | 13.9735 |
| data fitted to Wagner eq. |  |  |  | 121.8 | 21470 | B | 3441.40 |
|  |  |  |  | 126.6 | 25280 | C | -79.434 |
|  |  |  |  | 129.4 | 27750 | temp range 315-458 K |  |
|  |  |  |  | 133.4 | 31600 |  |  |
|  |  |  |  | 137.2 | 35660 |  |  |
|  |  |  |  | 141.9 | 41250 |  |  |



FIGURE 2.1.1.1.26.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-decane.

### 2.1.1.1.27 n-Undecane



Common Name: $n$-Undecane
Synonym: undecane
Chemical Name: $n$-undecane
CAS Registry No: 1120-21-4
Molecular Formula: $\mathrm{C}_{11} \mathrm{H}_{24} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{9} \mathrm{CH}_{3}$
Molecular Weight: 156.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-25.5 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 195.9 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.74024,0.73652 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Camin \& Rossini 1955) $0.7402,0.7366 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $211.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 251.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $56.5,41.524\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1959) 56.58 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $6.86,22.18,29.03 \quad\left(-36.55,-25.55^{\circ} \mathrm{C}\right.$, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 118.6, 119.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0044 (shake flask-GC, McAuliffe 1969)
0.0036 (shake flask-GC, Krashoshhchekova \& Gubertritis 1973)
0.0040 ("best" value, IUPAC Solubility Data Series, Shaw 1989)
0.0042 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$133.3^{*} \quad\left(31.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $31.4-194.5^{\circ} \mathrm{C}$, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97674-1572.477 /\left(188.022+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $105.4-197.3^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurement, Camin \& Rossini 1955)
57.18 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97674-1572.477 /\left(188.022+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $98-258^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
52.20* (extrapolated-Antoine eq., temp range $75.1-225.8^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97220-1569.57 /\left(187.700+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75.1-225.8^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \&
Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 11481.7 /(\mathrm{T} / \mathrm{K})]+8.260477$; temp range $31.4-194.5^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
52.5 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.12013-1572.031 /\left(188.062+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $104.5-197.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data of Camin \& Rossini 1955, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97220-1569.57 /\left(187.70+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-226^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
54.8 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.10154-1572.411 /(-85.128+\mathrm{T} / \mathrm{K})$; temp range $278-470 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
56.89* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.02771-2.045579 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.712658 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=469.042 \mathrm{~K}($ Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=82.9230-5.6085 \times 10^{3} /(\mathrm{T} / \mathrm{K})-23.7327 \cdot \log (\mathrm{~T} / \mathrm{K})+1.0469 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+7.087 \times 10^{-13} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $248-639 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
185000 (calculated-P/C, Mackay \& Shiu 1981)
185390 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
6.94 (estimated-HPLC/MS, Burkhard et al. 1985)
6.51 (calculated-fragment const., Burkhard et al. 1985)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=13.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=1.32 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}=1.29 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

TABLE 2.1.1.1.27.1
Reported vapor pressures of $n$-undecane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$ | (5) - Cox eq. |  |


| Stull 1947 |  | Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| 31.4 | 133.3 | 104.58 | 5540 | 75.1 | 1333 | 236.04 | 0.1 |
| 58.4 | 666.6 | 110.952 | 8287 | 89.06 | 2666 | 254.71 | 1.0 |
| 72.2 | 1333 | 115.522 | 8337 | 97.93 | 4000 | 277.39 | 10 |
| 86.3 | 2666 | 118.963 | 9358 | 104.58 | 5333 | 305.75 | 100 |
| 103.1 | 5333 | 122.607 | 10954 | 109.95 | 6666 | 342.64 | 1000 |
| 113.9 | 7999 | 127.467 | 13104 | 114.486 | 7999 | 393.33 | 10000 |
| 126.8 | 13332 | 132.757 | 15837 | 121.934 | 10666 | 469.04 | 101325 |

TABLE 2.1.1.1.27.1 (Continued)

| Stull 1947 |  | Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| 148.0 | 26664 | 138.713 | 19448 | 127.969 | 13332 | 298.15 | 56.89 |
| 170.6 | 53329 | 143.585 | 22889 | 139.559 | 19998 |  |  |
| 194.5 | 101325 | 150.437 | 28550 | 148.312 | 26664 | Cox eq. |  |
|  |  | $156.841$ | 34826 | $155.431$ | 33331 | eq. 5 | $\mathrm{P} / \mathrm{kPa}$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | 164.039 | 43031 | 161.475 | 39997 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
|  |  | 171.724 | 53780 | 171.458 | 53329 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 469.64 |
|  |  | 179.802 | 67077 | 179.603 | 66661 | a | 3.02711 |
|  |  | 188.431 | 84053 | 186.537 | 79993 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.045579 |
|  |  | 194.595 | 98132 | 192.608 | 93326 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.712658 |
|  |  | 195.242 | 101081 | 193.739 | 95992 |  |  |
|  |  | 196.511 | 102882 | 194.845 | 98659 |  |  |
|  |  | 197.272 | 104822 | 195.928 | 101325 |  |  |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 195.890 | bp/ ${ }^{\circ} \mathrm{C}$ | 195.928 |  |  |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  | A | 6.97674 | A | 6.97220 |  |  |
|  |  | B | 1572.477 | B | 1569.57 |  |  |
|  |  | C | 188.022 | C | 187.700 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  |
|  |  |  |  | $\text { at } 25^{\circ} \mathrm{C}$ | $56.34$ |  |  |
|  |  |  |  | at bp | 41.50 |  |  |



FIGURE 2.1.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-undecane.

### 2.1.1.1.28 <br> n-Dodecane



Common Name: $n$-Dodecane
Synonym: dodecane
Chemical Name: $n$-dodecane
CAS Registry No: 112-40-3
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{26} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{10} \mathrm{CH}_{3}$
Molecular Weight: 170.334
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-9.57 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
216.32 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.7487, $0.7452 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
$0.74941 \quad\left(20^{\circ} \mathrm{C}\right.$, densimeter, Dejoz et al. 1996)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$227.5 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
273.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
61.287, $43.64 \quad\left(25^{\circ}, \mathrm{bp}\right.$, Riddick et al. 1986)
$61.52 \quad$ (298.15 K, recommended, Ruzicka \& Majer 1994)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
36.84 (Dreisbach 1959)
35.86 (Riddick et al. 1986)
36.82 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
139.75, 128.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0084 (shake flask-GC, Franks 1966)
0.0034 (shake flask-GC, McAuliffe 1969)
0.0037 (shake flask-GC, Sutton \& Calder 1974)
0.0037 (recommended, IUPAC Solubility Data Series, Shaw 1989)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$6365^{*} \quad\left(126.31^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $126.31-217.345^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98059-1625.928 /\left(180.311+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $126.4-217.3^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
$133.3^{*} \quad\left(47.7^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $47.7-214.5^{\circ} \mathrm{C}$, Stull 1947)
17.60 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98059-1625.928 /\left(180.311+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $150-280^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
15.70* (extrapolated-Antoine eq., temp range $91.47-247.08^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
7.60 (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99795-1639.27 /\left(181.835+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $91.47-247.08^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 11857.7 /(\mathrm{T} / \mathrm{K})]+8.150997$; temp range $47.7-345.8^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 15.5 (Antoine eq., Boublik et al. 1973, 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9829-1627.714 /\left(180.521+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $104.5-197.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)
32.53 (calculated-bp, Mackay et al. 1982)
$\log (\mathrm{P} / \mathrm{kPa})=6.1074-1627.417 /\left(180.489+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $104.5-197.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99795-1639.27 /\left(181.84+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $91-247^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
17.3* $\quad\left(24.931^{\circ} \mathrm{C}\right.$, gas saturation, measured temp range $298.081-389.66 \mathrm{~K}$, Allemand et al. 1986)
16.0 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.12285-1639.27 /\left(181.835+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
18.6 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.62064-1942.122 /(-65.587+\mathrm{T} / \mathrm{K})$; temp range $278-400 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.12285-1639.27 /(-91.315+\mathrm{T} / \mathrm{K})$; temp range $400-492 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$18.40,18.67^{*}\left(25.30,25.35^{\circ} \mathrm{C}\right.$, electronic manometry, measured range -9.27 to $98.10^{\circ} \mathrm{C}$, Sasse et al. 1988)
$733.8^{*} \quad\left(79.969^{\circ} \mathrm{C}\right.$, static-differential pressure, measured range $79.969-314.982^{\circ} \mathrm{C}$, Morgan \& Kobayashi 1994)
18.02 (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.05854-2.018454 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.606849 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=489.438 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=-5.6532-3.4698 \times 10^{3} /(\mathrm{T} / \mathrm{K})+9.0272 \cdot \log (\mathrm{~T} / \mathrm{K})-2.3185 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+1.1235 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $264-658 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
14.1; 17.8 (liquid $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation; quoted lit., Donovan 1996)

440* (71.6 ${ }^{\circ} \mathrm{C}$, ebulliometry, measured range $344.25-501.55 \mathrm{~K}$, Dejoz et al. 1996)
$\ln (\mathrm{P} / \mathrm{kPa})=14.1090-3781.84 /[(\mathrm{T} / \mathrm{K})-90.975]$; temp range $344.25-501.55 \mathrm{~K}$ (ebulliometry, Dejoz et al. 1996)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
723000 (calculated-P/C, Bobra et al. 1979)
723000, 786000, 317000; 750000 (calculated-P/C values; recommended, Mackay \& Shiu 1981)
721400 (selected, Mills et al. 1982)
726900 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
7.24, 7.04 (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)
$6.10 \quad$ (Coates et al. 1985)
$6.80 \pm 1.00$ (recommended, Sangster 1989)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constant, k, and Half-Lives, $t_{1 / 2}$ :
Volatilization: rate constants: $\mathrm{k}=0.60 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=1.1 \mathrm{~d}$ in spring at $8-16^{\circ} \mathrm{C}, \mathrm{k}=0.97 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=0.7 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{k}=0.20 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=3.6 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ for the periods when volatilization appears to dominate, and $\mathrm{k}=0.377 \mathrm{~d}^{-1}$, $\mathrm{t}_{1 / 2}=1.8 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$, and $\mathrm{k}=1.085 \mathrm{~d}^{-1}$, $\mathrm{t}_{1 / 2}=0.64 \mathrm{~d}$ without $\mathrm{HgCl}_{2}$ in September 9-15, in marine mesocosm experiments (Wakeham et al. 1983)
Photolysis:
Oxidation: rate constant $k$ for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, ${ }^{*}$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=15.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=14.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}=13.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: Surface water: estimated $t_{1 / 2}=0.5 \mathrm{~d}$ for surface waters in case of first order reduction process (Zoeteman et al. 1980)
marine mesocosm $\mathrm{t}_{1 / 2}=1.1 \mathrm{~d}$ at $8-16^{\circ} \mathrm{C}$ in spring, $\mathrm{t}_{1 / 2}=0.7 \mathrm{~d}$ at $20-22^{\circ} \mathrm{C}$ in summer and $\mathrm{t}_{1 / 2}=3.6 \mathrm{~h}$ at $3-7^{\circ} \mathrm{C}$ in winter when volatilization dominates, and $\mathrm{t}_{1 / 2}=1.8 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ as poison, and $\mathrm{k}=1.085 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=0.64 \mathrm{~d}$ without poison in mid-September (Wakeham et al. 1983)

TABLE 2.1.1.1.28.1
Reported vapor pressures of $\boldsymbol{n}$-dodecane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$ | (5) -Coxeq. |  |

1. 

| Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  | Allemand et al. 1986 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | summary of literature data |  | selected values |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 126.31 | 6365 | 47.7 | 133.3 | 91.47 | 1333 | 24.931 | 17.33 |
| 131.108 | 7663 | 75.7 | 666.6 | 105.91 | 2666 | 28.95 | 24.66 |
| 135.223 | 8971 | 89.9 | 1333 | 115.09 | 4000 | 29.966 | 26.66 |
| 138.962 | 10306 | 104.3 | 2666 | 121.96 | 5333 | 35.043 | 40.00 |
| 142.444 | 11696 | 121.4 | 5333 | 127.521 | 6666 | 40.023 | 58.13 |
| 147.152 | 13816 | 131.7 | 7999 | 132.213 | 7999 | 40.29 | 60.26 |
| 152.529 | 16611 | 145.5 | 13332 | 139.915 | 10666 | 45.023 | 84.79 |
| 157.986 | 19917 | 165.8 | 26664 | 146.153 | 13332 | 49.978 | 120.5 |
| 163.030 | 23443 | 188.4 | 53329 | 158.131 | 19998 | 50.0 | 118.8 |
| 169.814 | 28948 | 214.5 | 101325 | 167.175 | 26664 | 55.32 | 170.7 |
| 176.039 | 34896 |  |  | 174.527 | 33331 | 59.936 | 232.0 |
| 183.537 | 43331 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -9.6 | 180.769 | 39997 | 64.936 | 310.6 |
| 191.255 | 53654 |  |  | 191.075 | 53329 | 69.23 | 409.3 |
| 199.488 | 66750 |  |  | 199.481 | 66661 | 70.093 | 422.6 |
| 208.417 | 83701 |  |  | 206.636 | 79993 | 74.947 | 558.6 |
| 214.709 | 97594 |  |  | 212.898 | 93326 | 78.83 | 691.9 |
| 215.303 | 99189 |  |  | 214.065 | 95992 | 80.174 | 745.3 |
| 216.006 | 100671 |  |  | 215.206 | 98659 | 99.87 | 2013 |
| 216.712 | 102385 |  |  | 216.323 | 101325 | 116.5 | 4258 |
| $217.345$ | 103910 |  |  |  |  |  |  |
|  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 216.323 |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 216.278 |  |  |  |  |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
| A | 6.98059 |  |  | A | 6.97220 |  |  |
| B | 1625.928 |  |  | B | 1639.27 |  |  |
| C | 180.311 |  |  | C | 181.835 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 61.59 |  |  |
|  |  |  |  |  | 43.64 |  |  |

TABLE 2.1.1.1.28.1 (Continued)
2.

| Sasse et al. 1988 |  |  |  | Dejoz et al. 1996 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| electronic manometry |  |  |  | vapor-liquid equilibrium |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| -9.27 | 0.587 | 92.17 | 1380 | 71.2 | 440 | 248.34 | 0.1 |
| -3.94 | 1.069 | 95.15 | 1599 | 75.6 | 570 | 267.74 | 1.0 |
| 0.49 | 1.720 | 98.10 | 1847 | 81.6 | 800 | 291.28 | 10 |
| 5.48 | 2.986 |  |  | 86.7 | 1040 | 320.68 | 100 |
| 5.53 | 2.920 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 91.1 | 1310 | 358.87 | 1000 |
| 10.47 | 4.800 | A | 1.17283 | 98.2 | 1860 | 411.27 | 10000 |
| 15.41 | 6.906 | B | 1766.802 | 102 | 2230 | 489.44 | 101325 |
| 15.46 | 7.706 | C | 194.662 | 106.8 | 2780 | 298.15 | 18.02 |
| 20.35 | 12.36 | Morgan \& Kobayashi 1994 |  | 111.2 | 3380 |  |  |
| 20.38 | 12.05 |  |  | 118.5 | 4430 | Cox eq. |  |
| 25.30 | 18.40 |  |  | 122.9 | 5540 | $\text { eq. } 5$ | P/kPa |
| 25.35 | 18.67 | static-differential pressure gauge |  | 126.5 | 6380 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
| 30.27 | 27.60 | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | 130.6 | 7520 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 489.438 |
| 30.30 | 28.13 |  |  | 135.2 | 8960 | a | 3.05854 |
| 35.27 | 40.80 | 79.969 | 733.8 | 143 | 11930 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.018454 |
| 35.30 | 41.33 | 99.970 | 2031 | 149.5 | 14980 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.606849 |
| 40.25 | 59.33 | 119.921 | 4912 | 154.8 | 17930 |  |  |
| 40.30 | 60.13 | 139.927 | 10690 | 160.8 | 21810 |  |  |
| 45.15 | 84.93 | 159.973 | 21248 | 166.1 | 25800 |  |  |
| 45.22 | 85.86 | 179.974 | 39125 | 171.0 | 29990 |  |  |
| 50.04 | 119.3 | 199.975 | 67572 | 175.7 | 34530 |  |  |
| 50.18 | 121.2 | 219.976 | 110500 | 180.8 | 40060 |  |  |
| 55.02 | 164.9 | 239.976 | 172410 | 183.3 | 42990 |  |  |
| 55.12 | 167.3 | 259.979 | 258710 | 186.0 | 46390 |  |  |
| 60.08 | 227.0 | 279.980 | 375270 | 189.8 | 51530 |  |  |
| 60.12 | 230.4 | 299.981 | 528820 | 193.2 | 56510 |  |  |
| 65.11 | 313.2 | 314.982 | 671130 | 197.6 | 63480 |  |  |
| 70.09 | 420.2 |  |  | 200.0 | 67570 |  |  |
| 75.08 | 558.4 | data fitt | gner eq. |  |  |  |  |
| 76.68 | 612.2 |  | see ref. | eq. 3(a) | $\mathrm{P} / \mathrm{kPa}$ |  |  |
| 80.12 | 735.8 |  |  | A | 14.1090 |  |  |
| 82.10 | 820.0 |  |  | B | 3781.84 |  |  |
| 85.11 | 949.1 |  |  | C | -90.975 |  |  |
| 87.26 | 1069 |  |  | temp ran | 5-502 K |  |  |



FIGURE 2.1.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-dodecane.

### 2.1.1.1.29 <br> n-Tridecane



Common Name: Tridecane
Synonym:
Chemical Name: $n$-tridecane
CAS Registry No: 629-50-5
Molecular Formula: $\mathrm{C}_{13} \mathrm{H}_{28} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{11} \mathrm{CH}_{3}$
Molecular Weight: 184.361
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -5.4 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 235.47 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ :
$0.76522,0.75270 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Camin \& Rossini 1955)
$0.7564,0.7528 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
296.0 (calculated-Le Bas method at normal boiling point)
$243.7 \quad\left(20^{\circ} \mathrm{C}\right.$, Stephenson \& Malanowski 1987)
Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $66.23,45.65\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986) 66.68 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $28.501 \quad$ (Riddick et al. 1986) 7.66, 28.49; $36.15 \quad\left(-18.15,-5.35^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 136.31, 137.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$133.3^{*} \quad\left(59.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $59.4-234.0^{\circ} \mathrm{C}$, Stull 1947)
5530* $\quad\left(139.3^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $139.3-236.065^{\circ} \mathrm{C}$, Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00339-1689.093 /\left(174.284+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $145.1-236.1^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Camin \& Rossini 1955)
5.30 (extrapolated-Antoine eq., Dreisbach 1959; quoted, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9887-1677.43 /\left(172.90+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $131-302^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
5.73* (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00756-1690.67 /\left(107.20+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $107.2-267.04^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 12991.3 /(\mathrm{T} / \mathrm{K})]+8.481732$; temp range $59.4-234^{\circ} \mathrm{C}$ (Antoine eq., Weast $197-73$ )
4.55 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
$\log \left(\mathrm{P} / \mathrm{mmHg}=7.00925-1693.684 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+174.815\right)\right.$; temp. range $139-236^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Camin \& Rossini 1955, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{kPa})=6.13542-1694.624 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+174.916\right)$; temp. range $139-236^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl data of Camin \& Rossini 1955, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00756-1690.67 /\left(174.22+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $107-267^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$
$\log (\mathrm{P} / \mathrm{kPa})=6.13246-1690.67 /\left(174.220+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) $\log (\mathrm{P} / \mathrm{mmHg})=7.00756-1690.67 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+174.22\right)$; temp range $107-267^{\circ} \mathrm{C}$, (Antoine eq., Dean 1985; 1992) $\log (\mathrm{P} / \mathrm{kPa})=6.13546-1690.67 /(\mathrm{T} / \mathrm{K}-98.93)$; temp range $417-511 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
5.682* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.10403-2.071819 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.61160 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=508.602 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=49.2391-4.9649 \times 10^{3} /(\mathrm{T} / \mathrm{K})-13.769 \cdot \log (\mathrm{~T} / \mathrm{K})-2.1146 \times 10^{-9} \cdot(\mathrm{~T} / \mathrm{K})+2.5902 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $268-676 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
233351 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
6.65 (HPLC-k' correlation, Coates et al. 1985)
6.50; 6.05 (calculated-fragment const.; calculated-molar volume, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $k$ for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=17.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=15.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $300 \mathrm{~K}, 17.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 302 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=16.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants $\left(\mathrm{k}_{1}\right.$ and $\left.\mathrm{k}_{2}\right)$ :
Half-Lives in the Environment:

TABLE 2.1.1.1.29.1
Reported vapor pressures of $\boldsymbol{n}$-tridecane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right.$ | (5) - Cox eq. |  |

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(5) - Cox eq.

Camin \& Rossini 1955
summary of literature data

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 59.4 | 133.3 |  | 139.3 | 5530 |
| 98.3 | 666.6 |  | 145.16 | 6931 |

Ruzicka \& Majer 1994 recommended

| T/K | $\mathbf{P} / \mathbf{P a}$ |
| :---: | :---: |
| 260.30 | 0.1 |
| 280.31 | 1.0 |

TABLE 2.1.1.1.29.1 (Continued)

| Stull 1947 |  | Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | T/K | P/Pa |
| 104.0 | 1333 | 150.011 | 8326 | 131.48 | 4000 | 304.58 | 10 |
| 120.2 | 2666 | 157.603 | 10934 | 138.55 | 5333 | 335.89 | 100 |
| 137.7 | 5333 | 162.749 | 13079 | 144.258 | 6666 | 374.24 | 1000 |
| 148.2 | 7999 | 174.699 | 19416 | 149.08 | 7999 | 428.21 | 10000 |
| 162.5 | 13332 | 187.176 | 28544 | 156.993 | 10666 | 508.60 | 101325 |
| 185.0 | 26664 | 201.634 | 43155 | 163.404 | 13332 | 298.15 | 5.682 |
| 209.4 | 53329 | 209.788 | 53768 | 175.709 | 19998 |  |  |
| 234.0 | 101325 | 218.367 | 67061 | 184.998 | 26664 | Cox eq. |  |
|  |  | 227.524 | 84040 | 192.55 | 33331 | $\text { eq. } 5$ | $\mathrm{P} / \mathrm{kPa}$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -6.2 | 234.052 | 85041 | 198.96 | 39997 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
|  |  | 235.316 | 101054 | 209.543 | 53329 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 469.64 |
|  |  | 236.065 | 102829 | 218.175 | 66661 | a | 3.10403 |
|  |  |  |  | 225.521 | 79993 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.071819 |
|  |  |  |  | 231.95 | 93326 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.712658 |
|  |  |  |  | $233.148$ | $95992$ |  |  |
|  |  |  |  | $234.319$ | $98659$ |  |  |
|  |  |  |  | 235.466 | 101325 |  |  |
|  |  |  |  | 25.0 | 5.73 |  |  |
|  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 235.466 |  |  |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  |  |  | A | 7.00756 |  |  |
|  |  |  |  | B | 1690.67 |  |  |
|  |  |  |  | C | 174.220 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}}$ | $\left.\mathrm{ol}^{-1}\right)=$ |  |  |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 66.23 |  |  |
|  |  |  |  | at bp | 45.65 |  |  |



FIGURE 2.1.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-tridecane.

### 2.1.1.1.30 <br> n-Tetradecane



Common Name: Tetradecane
Synonym:
Chemical Name: $n$-tetradecane
CAS Registry No: 629-59-4
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{30} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{12} \mathrm{CH}_{3}$
Molecular Weight: 198.388
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): $5.82 \quad$ (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 253.58 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ): $0.76275,0.75917 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Camin \& Rossini 1955) $0.7628,0.7593 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$260.1 \quad\left(20^{\circ} \mathrm{C}\right.$, Stephenson \& Malanowski 1987)
318.2 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$71.13,47.73\left(25^{\circ} \mathrm{C}\right.$, bp, Dreisbach 1961)
71.73 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 45.07 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 161.54, 147.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0069 (shake flask-GC, Frank 1966)
0.00655 (extrapolated, McAuliffe 1966)
0.0022; 0.0017 (shake flask-GC, distilled water; seawater, Sutton \& Calder 1974)
0.00033 (shake flask-GC, Coates et al. 1985)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$133.3^{*} \quad\left(76.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $76.4-252.5^{\circ} \mathrm{C}$, Stull 1947)
$5532^{*} \quad\left(154.860^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $154.860-254.165^{\circ} \mathrm{C}$, Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01245-1739.623 /\left(167.534+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $165.9-254.2^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Camin \& Rossini 1955)
1.56 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9957-1725.46 /\left(165.75+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $147-325^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
1.27* (Antoine eq., temp range $121.80-286.0^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
1.867 (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01300-1740.88 /\left(167.720+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $121.80-286.0^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 13750.0 /(\mathrm{T} / \mathrm{K})]+8.628699$; temp range $76.4-252.5^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
1.30 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02216-1747.452 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+168.437\right)$; temp range $155-254^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Camin \& Rossini 1955, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{kPa})=6.14914-1749.052 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+168.611\right)$; temp range $155-254^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Camin \& Rossini 1955, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01300-1740.88 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+167.72\right)$; temp. range $112-286^{\circ} \mathrm{C}$ (Antoine eq., Dean $1985 ; 1992$ ) 72.0* $\quad\left(70.01^{\circ} \mathrm{C}\right.$, gas saturation, measured temp range $343.16-394.73 \mathrm{~K}$, Allemand et al. 1986)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.62828-2063.84 /(\mathrm{T} / \mathrm{K}-77.378)$; temp range $313-433 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1379-1740.88 /(\mathrm{T} / \mathrm{K}-105.43)$; temp. range $432-529 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
442.9* $\quad\left(99.926^{\circ} \mathrm{C}\right.$, static-differential pressure, measured range $99.926-314.982^{\circ} \mathrm{C}$, Morgan \& Kobayashi 1994)
1.804* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.13624-2.063853 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.541507 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=526.691 \mathrm{~K}($ Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=106.1056-7.3461 \times 10^{3} /(\mathrm{T} / \mathrm{K})-31.5195 \cdot \log (\mathrm{~T} / \mathrm{K})+1.2356 \times 10^{-2} .(\mathrm{T} / \mathrm{K})-8.3955 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2}$; temp range 279-692 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
347000 (calculated-P/C, Mackay \& Shiu 1981)
387000 (calculated-P/C, Eastcott et al. 1988)
114497 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
7.20 (HPLC-k' correlation, Coates et al. 1985)
7.88, 8.10 (RP-HPLC-MS correlation, Burkhard et al. 1985)
7.00; 6.45 (calculated-fragment const.; calculated-molar volume, Wang et al. 1992)
8.0 (recommended, Sangster 1989, 1993)
6.49 (calculated-UNIFAC, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=19.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=19.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=19.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=18.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<15 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:

TABLE 2.1.1.1.30.1
Reported vapor pressures of $n$-tetradecane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
(3)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4)
$\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$
(5) - Cox eq.
1.

| Stull 1947 |  | Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  | Allemand et al. 1986 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
| 76.4 | 133.3 | 154.860 | 5532 | 121.8 | 1333 | 70.01 | 71.99 |
| 106.0 | 666.6 | 165.911 | 6325 | 137.06 | 2666 | 70.45 | 74.53 |
| 120.7 | 1333 | 173.737 | 10928 | 146.75 | 4000 | 80.0 | 136.8 |
| 135.6 | 2666 | 191.234 | 19417 | 154.01 | 5333 | 91.0 | 262.7 |
| 152.7 | 5333 | 204.019 | 28546 | 159.881 | 6666 | 106.78 | 634.6 |
| 164.0 | 7999 | 218.84 | 43156 | 164.836 | 7999 | 121.58 | 1324 |
| 178.5 | 13332 | 236.013 | 67061 | 172.967 | 10666 |  |  |
| 201.8 | 26664 | 245.408 | 84041 | 179.553 | 13332 |  |  |
| 226.8 | 53329 | 252.104 | 98106 | 192.196 | 19998 |  |  |
| 252.5 | 101325 | 253.401 | 101061 | 201.739 | 26664 |  |  |
|  |  | 254.165 | 102850 | 209.497 | 33331 |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 5.5 |  |  | 216.082 | 39997 |  |  |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 253.516 | 226.953 | 53329 |  |  |
|  |  |  |  | $235.819$ | $66661$ |  |  |
|  |  |  |  | $243.364$ | $79993$ |  |  |
|  |  |  |  | 249.967 | 93326 |  |  |
|  |  |  |  | 251.197 | 95992 |  |  |
|  |  |  |  | 252.4 | 98659 |  |  |
|  |  |  |  | 253.577 | 101325 |  |  |

TABLE 2.1.1.1.30.1 (Continued)
2.

| Morgan \& Kobayashi 1994 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: |
| differential pressure gauge |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathrm{P} / \mathrm{Pa}$ |
| 99.926 | 442.9 | 271.60 | 0.1 |
| 119.936 | 1227 | 292.22 | 1.0 |
| 139.946 | 3026 | 317.21 | 10 |
| 159.956 | 6693 | 348.38 | 100 |
| 179.965 | 13526 | 388.82 | 1000 |
| 199.976 | 25267 | 444.22 | 10000 |
| 219.976 | 44274 | 526.69 | 101325 |
| 229.964 | 57442 | 298.15 | 1.804 |
| 239.977 | 73530 |  |  |
| 249.979 | 93059 | Cox eq. |  |
| 259.979 | 116500 | eq. 5 | P/kPa |
| 249.979 | 116520 | $\mathrm{P}_{\text {ref }} / \mathrm{KPa}$ | 101.325 |
| 279.980 | 177570 | $\mathrm{T}_{\text {ree }} / \mathrm{K}$ | 526.691 |
| 299.980 | 261560 | a | 3.13624 |
| 309.982 | 314050 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.063853 |
| 314.982 | 343450 | $10^{6} / \mathrm{K}^{-2}$ | 1.541507 |

data fitted to Wagner eq.


FIGURE 2.1.1.1.30.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-tetradecane.

### 2.1.1.1.31 n-Pentadecane



Common Name: Pentadecane
Synonym:
Chemical Name: n-pentadecane
CAS Registry No: 629-62-9
Molecular Formula: $\mathrm{C}_{15} \mathrm{H}_{32} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{13} \mathrm{CH}_{3}$
Molecular Weight: 212.415
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
9.95 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
270.6 (Camin \& Rossini 1955; Dreisbach 1959; Stephenson \& Malanowski 1987; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ :
0.76830, $0.76488\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Camin \& Rossini 1955)
$0.7685,0.7650\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$276.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
340.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
76.16, $49.41\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1961)
76.77 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.17, 34.6; 43.77 ( $-2.25,9.95$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
156.02, 156.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
$7.6 \times 10^{-5}$ (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
0.0612; 0.0613 (measured; calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
133.3* $\quad\left(91.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $91.6-270.5^{\circ} \mathrm{C}$, Stull 1947)

5532* ( $169.686^{\circ} \mathrm{C}$, ebulliometry, measured range $169.686-270.449^{\circ} \mathrm{C}$, Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02445-1789.658 /\left(161.291+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $169.6-270.6^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Camin \& Rossini 1955)
0.311 (extrapolated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0017-1768.82 /\left(158.60+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $160-338^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

1333* $\quad\left(135.8^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $135.8-270.685^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971) $\log (\mathrm{P} / \mathrm{mmHg})=7.01359-1789.95 /\left(161.380+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $135.8-303.8^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 14635.9 /(\mathrm{T} / \mathrm{K})]+8.822087$; temp range $91.6-270.5^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
0.356 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log \mathrm{P} / \mathrm{mmHg}=7.03121-1797.239 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+164.128\right.$ ); temp range $170-270^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data of Camin \& Rossini 1955, Boublik et al. 1973)
0.359 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.15888-1797.239 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+162.128\right)$; temp range $170-270.5^{\circ} \mathrm{C}$ (Antoine eq. derived from exptl. data of Camin \& Rossini 1955, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02359-1789.95 /\left(161.38+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $136-304^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$15.87^{*} \quad\left(60.0^{\circ} \mathrm{C}\right.$, gas saturation, measured temp range $60.0-136.0^{\circ} \mathrm{C}$, Allemand et al. 1986)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.38149-1945.469 /(\mathrm{T} / \mathrm{K}-97.875)$; temp range $366-409 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.14849-1789.95 /(\mathrm{T} / \mathrm{K}-111.77)$; temp range $447-546 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
0.576* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.16144-2.062348 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.487263 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=543.797 \mathrm{~K}($ Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=116.5157-8.041 \times 10^{3} /(\mathrm{T} / \mathrm{K})-38.799 \cdot \log (\mathrm{~T} / \mathrm{K})-1.3398 \times 10^{-2} .(\mathrm{T} / \mathrm{K})-4.4444 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $283-707 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
48535 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
7.72 (HPLC-k' correlation, Coates et al. 1985)
7.50; 6.78 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constant, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: volatilization rate constant of $\mathrm{k}=0.69 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=1.0 \mathrm{~d}$ at $6-18^{\circ} \mathrm{C}$, in spring; $\mathrm{k}=0.85 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=0.8 \mathrm{~d}$ at $20-22^{\circ} \mathrm{C}$ in summer; $\mathrm{k}=0.16 \mathrm{~d}^{-1}$ with a water column $t_{1 / 2}=4.3 \mathrm{~d}$ at $3-7^{\circ} \mathrm{C}$ in winter for mesocosm experiment in coastal marine environment when volatilization dominates, volatilization $\mathrm{k}=0.343 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=2.0 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ poisoned water tank and $\mathrm{k}=1.241 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=0.56 \mathrm{~d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=22.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=22.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=22.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=22.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (experimental); $17.87 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atmospheric Oxidation Program); and $7.47 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Fate of Atmospheric Pollutants) for gas-phase reaction with OH radicals (Meylan \& Howard 1993)
$\mathrm{k}_{\mathrm{OH}}=21.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<15 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants $\left(\mathrm{k}_{1}\right.$ and $\left.\mathrm{k}_{2}\right)$ :
Half-Lives in the Environment:
Surface water: water column half-lives, $\mathrm{t}_{1 / 2}=1.0 \mathrm{~d}, 6-18^{\circ} \mathrm{C}$, in spring; $\mathrm{t}_{1 / 2}=0.8 \mathrm{~d}, 20-22^{\circ} \mathrm{C}$, in summer; $\mathrm{t}_{1 / 2}=4.3 \mathrm{~d}$, $3-7^{\circ} \mathrm{C}$, in winter for mesocosm experiment in coastal marine mesocosm; $\mathrm{t}_{1 / 2}=2.0 \mathrm{~d}$ with HgCl poisoned water tank and $t_{1 / 2}=0.56 \mathrm{~d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

TABLE 2.1.1.1.31.1
Reported vapor pressures of n-pentadecane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$ | (5) - Coxeq. |  |

Stull 1947

| summary of literature data |  |  |  |
| :---: | :---: | :---: | ---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  | $\mathbf{t} /{ }^{\circ} \mathrm{Ca}$ |
| 91.6 | 133.3 |  | 169 |
| 121.0 | 666.6 |  | 180.9 |
| 135.4 | 1333 |  | 188.9 |
| 150.2 | 2666 |  | 206.88 |
| 167.7 | 5333 |  | 219 |
| 178.4 | 7999 |  | 235 |
| 194.0 | 13332 |  | 151 |
| 216.1 | 26664 |  | 262 |
| 242.8 | 53329 |  | 269 |
| 270.5 | 101325 |  | 270 |
|  |  |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 10 |  |  |
|  |  |  |  |



FIGURE 2.1.1.1.31.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-pentadecane.

### 2.1.1.1.32 <br> n-Hexadecane



Common Name: Hexadecane
Synonym: cetane
Chemical Name: $n$-hexadecane
CAS Registry No: 544-76-3
Molecular Formula: $\mathrm{C}_{16} \mathrm{H}_{34} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{14} \mathrm{CH}_{3}$
Molecular Weight: 226.441
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
18.12 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
286.86 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.77344,0.76996\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Camin et al. 1954; Dreisbach 1959)
$0.7733 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$292.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
362.2 (calculated-Le Bas molar volume at normal boiling point, Eastcott et al. 1988)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
81.35 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $53.35,51.46 ; 53.35\left(18.15,17.95^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
$176.79,165.8$ (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ : $6.28 \times 10^{-3} \quad$ (shake flask, Franks 1966) $2.1 \times 10^{-5} \quad$ (extrapolated data of McAuliffe 1966, Coates et al. 1985) $5.21 \times 10^{-5} \quad$ (extrapolated from data of McAuliffe 1996, Eastcott et al. 1988) $9.0 \times 10^{-4}, 4.0 \times 10^{-4}$ (shake flask-GC, distilled water; seawater, Sutton \& Calder 1974) $2.33 \times 10^{-6} \quad$ (calculated-TSA, Lande et al. 1985)
0.0272 (calculated-molar volume correlation, Wang et al. 1992)
$4.95 \times 10^{-5} \quad$ (calculated-molar volume and mp., Ruelle Kesselring 1997)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
133.3* $\quad\left(105.3^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $105.3-287.5^{\circ} \mathrm{C}$, Stull 1947)
$6945^{*} \quad\left(190.054^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $190.054-286.704^{\circ} \mathrm{C}$, Camin et al. 1954)
$13.33^{*} \quad\left(81.0^{\circ} \mathrm{C}\right.$, static method -Hg manometer, measured range $81.0-286.0^{\circ} \mathrm{C}$, Myers \& Fenske 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03044-1831.317 /\left(154.528+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $190.0-286.8^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Camin et al. 1954)
$0.14 \quad\left(71.87^{\circ} \mathrm{C}\right.$, calculated-Antoine eq., Dreisbach 1959)
$0.221^{*} \quad$ (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02867-1830.51 /\left(154.450+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $149.18-320.7^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 15405.5 /(\mathrm{T} / \mathrm{K})]+8.956267$; temp range $105.3-287.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
0.092 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03519-1835.24 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+154.968\right)$; temp range $188-285^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data of Camin et al. 1945, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{kPa})=6.16189-1836.287 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+155.125\right)$; temp range $190-287^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data of Camin et al. 1954, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02867-1830.51 /\left(154.45+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $149-321^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.77064-2273.168 /(\mathrm{T} / \mathrm{K}-80.252)$; temp range $323-425 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.15357-1830.57 /(\mathrm{T} / \mathrm{K}-118.7)$; temp range $467-563 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02967-1830.51 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+154.45\right)$; temp range $149-321^{\circ} \mathrm{C}$ (Antoine eq., Dean 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=99.1091-7.5333 \times 10^{3} /(\mathrm{T} / \mathrm{K})-32.251 \cdot \log (\mathrm{~T} / \mathrm{K})+1.0453 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.2328 \times 10^{-12} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $291-721 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$317.6^{*} \quad\left(119.896^{\circ} \mathrm{C}\right.$, static-differential pressure, measured range $119.896-309.982^{\circ} \mathrm{C}$, Morgan \& Kobayashi 1994)
0.191* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.18271-2.002545 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+1.384476 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=559.978 \mathrm{~K}($ Cox equation, Ruzicka \& Majer 1994)
0.190 (GC-retention time correlation, Chickos \& Hanshaw 2004)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
389000 (calculated-P/C, Eastcott et al. 1988)
23072 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
8.25 (HPLC-k' correlation, Coates et al. 1985)
8.00; 7.26 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=25.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 312 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=25.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=23.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<31$ d by Pseudomonas sp. (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants $\left(\mathrm{k}_{1}\right.$ and $\left.\mathrm{k}_{2}\right)$ :
Half-Lives in the Environment:

## TABLE 2.1.1.1.32.1

Reported vapor pressures of $n$-hexadecane at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{aligned}
& \log P=A-B /(T / K) \\
& \log P=A-B /\left(C+t /{ }^{\circ} C\right) \\
& \log P=A-B /(C+T / K) \\
& \log P=A-B /(T / K)-C \cdot \log (T / K) \\
& \ln \left(P / P_{\text {ref }}\right)=\left[1-\left(T_{\text {ref }} / T\right)\right] \cdot \exp \left(a+b T+\mathrm{cT}^{2}\right.
\end{aligned}
$$

$\begin{array}{ll}\text { (1) } & \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\ \text { (2) } & \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\end{array}$
(2)
(3)
(4)
(5) - Cox eq.
1.

| Stull 1947 |  | Camin et al. 1954 |  | Myers \& Fenske 1955 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | static method-Hg manometer |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 105.3 | 133.3 | 190.054 | 6945 | 81.0 | 13.33 | 149.18 | 1333 |
| 135.2 | 666.6 | 193.301 | 8330 | 94.2 | 66.66 | 165.14 | 2666 |
| 149.8 | 1333 | 199.273 | 9351 | 105.3 | 133.3 | 175.28 | 4000 |
| 164.7 | 2666 | 203.437 | 10951 | 117.2 | 266.6 | 182.87 | 5333 |
| 181.2 | 5333 | 208.962 | 13098 | 124.9 | 400.0 | 189.00 | 6666 |
| 193.2 | 7999 | 215.00 | 15824 | 130.7 | 533.3 | 194.184 | 7999 |
| 208.5 | 13332 | 221.78 | 19448 | 135.5 | 666.6 | 202.682 | 10666 |
| 231.7 | 26664 | 227.336 | 22886 | 138.2 | 799.9 | 209.565 | 13332 |
| 258.3 | 53329 | 235.145 | 28558 | 145.0 | 1067 | 222.774 | 19998 |
| 287.5 | 101325 | 242.432 | 34817 | 150.0 | 1333 | 232.743 | 26664 |
|  |  | 250.605 | 43171 | 159.5 | 2000 | 240.846 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 18.5 | 259.336 | 53777 | 166.0 | 2666 | 247.723 | 39997 |
|  |  | 268.540 | 67076 | 176.0 | 4000 | 259.074 | 53329 |
|  |  | 278.333 | 84.065 | 183.6 | 5333 | 268.33 | 66661 |
|  |  | 285.337 | 98168 | 189.7 | 6666 | 276.205 | 79993 |
|  |  | 286.704 | 101325 | 194.3 | 7999 | 283.097 | 93326 |
|  |  |  |  | 202.6 | 10666 | 284.38 | 95992 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 286.792 | 209.8 | 13332 | 285.635 | 98659 |
|  |  |  |  | 222.3 | 19998 | 286.864 | 101325 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 232.2 | 26664 | 25.0 | 0.221 |
|  |  | A | 7.03044 | 245.8 | 39997 | bp/ ${ }^{\circ} \mathrm{C}$ | 286.854 |
|  |  | B | 1831.317 | 258.0 | 53329 |  |  |
|  |  | C | 154.528 | 267.0 | 66661 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  | 274.5 | 79993 | A | 7.02867 |
|  |  |  |  | 282.2 | 93326 | B | 1830.51 |
|  |  |  |  | 286.0 | 101325 | C | 154.450 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{k}$ | $\left.\mathrm{ol}^{-1}\right)=$ |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 81.09 |
|  |  |  |  |  |  | at bp | 51.21 |

TABLE 2.1.1.1.32.1 (Continued)
2.

| Morgan \& Kobayashi 1994 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: |
| static method pressure gauge |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathrm{P} / \mathrm{Pa}$ |
| 119.896 | 317.6 | 292.41 | 0.1 |
| 129.903 | 541.2 | 314.20 | 1.0 |
| 139.909 | 886.1 | 340.55 | 10 |
| 149.916 | 1408 | 373.36 | 100 |
| 159.929 | 2172 | 415.82 | 1000 |
| 169.929 | 3273 | 473.84 | 10000 |
| 179.935 | 4810 | 559.98 | 101325 |
| 189.943 | 6912 | 298.15 | 0.191 |
| 199.976 | 9774 |  |  |
| 209.956 | 13530 | Cox eq. |  |
| 219.976 | 18418 | eq. 5 | P/kPa |
| 229.969 | 24691 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
| 239.977 | 32600 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 469.64 |
| 249.979 | 42464 | a | 3.18271 |
| 259.979 | 54642 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.002545 |
| 269.979 | 69438 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.384476 |
| 279.980 | 87294 |  |  |
| 289.980 | 108620 |  |  |
| 299.980 | 133940 |  |  |
| 309.982 | 163530 |  |  |

data fitted to Wagner eq.


FIGURE 2.1.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-hexadecane.

### 2.1.1.1.33 n-Heptadecane



Common Name: Heptadecane
Synonym:
Chemical Name: $n$-heptadecane
CAS Registry No: 629-78-7
Molecular Formula: $\mathrm{C}_{17} \mathrm{H}_{36} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{15} \mathrm{CH}_{3}$
Molecular Weight: 240.468
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
22 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
302 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.7780,0.7745\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
0.7780 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
384.8 (calculated-Le Bas method at normal boiling point)
$309.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$61.65,53.12\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1961)
86.47 (298.15 K, recommended, Ruzicka \& Majer 1994)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 10.96, $40.17 ; 51.13\left(1.15,21.95^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
174.61, 175.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al.1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
$\begin{array}{ll}5.5 \times 10^{-6} & \text { (extrapolated from data of McAuliffe 1966, Coates et al. 1985) } \\ 0.0014 & \text { (reported as }-\log S(\mathrm{~mol} / \mathrm{L})=7.24 \text {, calculated-molar volume, Wang et al. 1992) }\end{array}$
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$1467^{*} \quad\left(163.5^{\circ} \mathrm{C}\right.$, temp range $163.5-303.0^{\circ} \mathrm{C}$, Krafft 1882 ; quoted, Boublik et al. 1984)
$133.3^{*} \quad\left(115.0^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $115.0-303.0^{\circ} \mathrm{C}$, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0115-1847.82 /\left(145.52+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $188-374^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
$0.0253^{*} \quad$ (derived from compiled data, temp range $160.9-337^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0143-1865.1 /\left(149.20+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $160.9-337^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 15608.5 /(\mathrm{T} / \mathrm{K})]+8.847487$; temp range $115-303^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 0.030 (extrapolated-Antoine eq., Boublik et al. 1973, 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97509-1851.699 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+149.263\right)$; temp range $164-303^{\circ} \mathrm{C}$ (Antoine eq., Boublik et al. 1973) $\log (\mathrm{P} / \mathrm{kPa})=6.09247-1845.726 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+148.633\right)$; temp range $164-303^{\circ} \mathrm{C}$ (Antoine eq., Boublik et al. 1984) $\log (\mathrm{P} / \mathrm{mmHg})=7.10143-1865.1 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+149.20\right)$; temp range $161-337^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
0.015 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=11.1197-4757.087 /(\mathrm{T} / \mathrm{K})$; temp range $289-320 \mathrm{~K}$ (Antoine eq.-I, liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1392-1865.1 /(\mathrm{T} / \mathrm{K}-123.95)$; temp range $488-577 \mathrm{~K}$ (Antoine eq.-II, liquid, Stephenson \& Malanowski 1987)
0.06148* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \_\exp \left\{3.21826-2.036553 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+1.383899 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=575.375 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=173.4039-1.0943 \times 10^{4} /(\mathrm{T} / \mathrm{K})-59.212 \cdot \log (\mathrm{~T} / \mathrm{K})+2.0705 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})-1.3433 \times 10^{-12} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $295-733 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
0.0627 (GC-retention time correlation, Chickos \& Hanshaw 2004)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
5415 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
8.92; 9.69 (estimated-RP-HPLC-MS; calculated-CLOGP, Burkhard et al. 1985)
8.79 (HPLC-k' correlation, Coates et al. 1985)
8.50; 7.68 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constant, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: volatilization $\mathrm{k}=1.23 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=0.6 \mathrm{~d}$ at $6-18^{\circ} \mathrm{C}$ in spring; $\mathrm{k}=0.79 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=0.9 \mathrm{~d}$ at $20-22^{\circ} \mathrm{C}$ in summer; $\mathrm{k}=0.14 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=5.0 \mathrm{~d}$ at $3-7^{\circ} \mathrm{C}$ in winter for mesocosm experiments in coastal marine environment; volatilization $k=0.359 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=1.9 \mathrm{~d}$ with HgCl poisoned water tank and $\mathrm{k}=1.362 \mathrm{~d}^{-1}$ with a water column $\mathrm{t}_{1 / 2}=0.51 \mathrm{~d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).
Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<31 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:
Surface water: water column $\mathrm{t}_{1 / 2}=0.6 \mathrm{~d}$ at $6-18^{\circ} \mathrm{C}$, in spring; $\mathrm{t}_{1 / 2}=0.9 \mathrm{~d}$ at $20-22^{\circ} \mathrm{C}$, in summer; $\mathrm{t}_{1 / 2}=5.0 \mathrm{~d}$ at $3-7^{\circ} \mathrm{C}$, in winter for mesocosm experiment in coastal marine environment; $\mathrm{t}_{1 / 2}=1.9 \mathrm{~d}$ with HgCl poisoned water tank and $t_{1 / 2}=0.51 \mathrm{~d}$ for non-poisoned water tank in late summer (Wakeham et al. 1983).

TABLE 2.1.1.1.33.1
Reported vapor pressures of $n$-heptadecane at various temperatures and the coefficients for the vapor pressure equations


TABLE 2.1.1.1.33.1 (Continued)

| Stull 1947 |  | Krafft 1882 |  | Zwolinski \& Wilhoit 1971 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | in Boublik et al. 1984 |  | selected values |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | T/K | $\mathbf{P / P a}$ |
| 207.3 | 7999 | 303.0 | 101325 | 207 | 7999 | 487.59 | 10000 |
| 223.0 | 13332 |  |  | 215.7 | 10666 | 575.38 | 101325 |
| 247.8 | 26664 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 303.003 | 222.76 | 13332 | 298.15 | 0.06148 |
| 274.5 | 53329 |  |  | 236.30 | 19998 |  |  |
| 303.0 | 101325 |  |  | 246.50 | 26664 | Cox eq. |  |
|  |  |  |  | 254.82 | 33331 | eq. 5 | $\mathrm{P} / \mathrm{kPa}$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 22.5 |  |  | 261.87 | 39997 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
|  |  |  |  | 273.51 | 53329 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 469.64 |
|  |  |  |  | 283.0 | 66661 | a | 3.21826 |
|  |  |  |  | 291.08 | 79993 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.036553 |
|  |  |  |  | 298.14 | 93326 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.383899 |
|  |  |  |  | 299.47 | 95992 |  |  |
|  |  |  |  | 300.76 | 98659 |  |  |
|  |  |  |  | 302.02 | 101325 |  |  |
|  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 302.02 |  |  |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  |  |  | A | 7.0143 |  |  |
|  |  |  |  | B | 1865.10 |  |  |
|  |  |  |  | C | 149.20 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ}$ |  |  |  |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 86.20 |  |  |
|  |  |  |  | at bp | 52.89 |  |  |



FIGURE 2.1.1.1.33.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-heptadecane.

### 2.1.1.1.34 n-Octadecane



Common Name: Octadecane
Synonym:
Chemical Name: $n$-octadecane
CAS Registry No: 543-45-3
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{38} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{16} \mathrm{CH}_{3}$
Molecular Weight: 254.495
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
28.2 (Dreisbach 1959; Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 316.3 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.7819,0.7785 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
0.7768 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$325.5 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
407.0 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

Enthalpy of vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
90.824, $54.84 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1959)
$91.6 \quad\left(25^{\circ} \mathrm{C}\right.$, Piacente et al. 1994)
$91.44 \quad$ (298.15K, recommended, Ruzicka \& Majer 1994)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
61.384 (Dreisbach 1959)
$61.13 \quad\left(28^{\circ} \mathrm{C}\right.$, Piacente et al. 1994)
61.5 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
204.6, 184.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.930\left(\mathrm{mp}\right.$ at $28.2^{\circ} \mathrm{C}$ )

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
$7.75 \times 10^{-3} \quad$ (Baker 1959)
$2.1 \times 10^{-3} ; 8.0 \times 10^{-4}$ (shake flask-GC, distilled water; seawater, Sutton \& Calder 1974)
$1.40 \times 10^{-6} \quad$ (extrapolated from data of McAuliffe 1966, Coates et al. 1988)
$4.05 \times 10^{-6} \quad$ (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$133.3^{*} \quad\left(119.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $119.6-317.0^{\circ} \mathrm{C}$, Stull 1947$)$
26.66* $\quad\left(102.4^{\circ} \mathrm{C}\right.$, static method- Hg manometer, measured range $102.4-313^{\circ} \mathrm{C}$, Myers \& Fenske 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0156-1883.73 /\left(139.46+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $201-387^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

1333* $\quad\left(172.3^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $172.3-316.3^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971$)$
$\log (\mathrm{P} / \mathrm{mmHg})=7.0022-1894.3 /\left(143.3+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $172.3-352^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 15447.0 /(\mathrm{T} / \mathrm{K})]+8.619864$; temp range $119.6-317^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 0.013 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.14067-2012.745 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+155.492\right)$; temp range $174-317^{\circ} \mathrm{C}$ (Antoine eq., Boublik et al. 1973) 0.0259 (liquid $P_{L}$, extrapolated-Antoine eq., Macknick \& Prausnitz 1979)
$0.220^{*} \quad\left(45.0^{\circ} \mathrm{C}\right.$, gas saturation, measured range $45.0-88.10^{\circ} \mathrm{C}$, Macknick \& Prausnitz 1979)
$\ln \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=25.548-10165 /(\mathrm{T} / \mathrm{K})$; temp range $45-88.1^{\circ} \mathrm{C}$ (Antoine eq. on exptl. data, gas saturation, liquid state, Macknick \& Prausnitz 1979)
0.0133 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.27065-2016.983 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+155.924\right)$; temp range $174-317^{\circ} \mathrm{C}$ (Antoine eq., Boublik et al. 1984) $\log (\mathrm{P} / \mathrm{mmHg})=7.0022-1894.3 /\left(143.30+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $172-352^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$1.15^{*} \quad\left(62.04^{\circ} \mathrm{C}\right.$, gas saturation, measured temp range $335.19-439.82 \mathrm{~K}$, Allemand et al. 1986)
0.0261 (extrapolated-Antoine eq.-I, liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=10.18833-4404.095 /(\mathrm{T} / \mathrm{K})$; temp range $310-361 \mathrm{~K}$ Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1392-1894.3 /(\mathrm{T} / \mathrm{K}-129.85)$; temp range $501-550 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0022-1894.3 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+143.30\right)$; temp range $172-352^{\circ} \mathrm{C}$ (Antoine eq., Dean 1992)
$256.6^{*} \quad\left(139.919^{\circ} \mathrm{C}\right.$, static-differential pressure, measured range $139.919-314.982^{\circ} \mathrm{C}$, Morgan \& Kobayashi 1994)
0.02007* (recommended, temp range 396-500 K, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.24741-2.048039 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+1.362445 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=590.023 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=-15.0772-4.8702 \times 10^{3} /(\mathrm{T} / \mathrm{K})+14.501 \cdot \log (\mathrm{~T} / \mathrm{K})-3.1625 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+1.3478 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $273-591 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa•m ${ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$1013 \quad\left(15^{\circ} \mathrm{C}\right.$, Wakeham et al. 1986)
622200 (calculated-P/C, Eastcott et al. 1988)
893 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
9.32 (HPLC-k' correlation, Coates et al. 1985)
9.00; 8.13 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
$5.90 \quad\left(\mathrm{~K}_{\mathrm{OM}}\right.$, Wakeham et al. 1986)
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization: volatilization rate constant $\mathrm{k}_{\mathrm{v}}=0.03 \mathrm{~d}^{-1}$, microcosm exptl. (Wakeham et al. 1986).
Photolysis:
Photooxidation:
Hydrolysis:
Biodegradation: degradation rate constant of about $0.66 \mathrm{~d}^{-1}$ in a microcosm expt. (Wakeham et al. 1986); microbial degradation $\mathrm{t}_{1 / 2}<31 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993).
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:
Surface water: an estimated $t_{1 / 2}=1.5 \mathrm{~d}$ in Rhine River for a first order reduction process in river water (Zoeteman et al. 1980)
$t_{1 / 2} \sim 23 \mathrm{~d}$ in a seawater microcosm experiment (Wakeham et al. 1986).

TABLE 2.1.1.1.34.1
Reported vapor pressures of $\boldsymbol{n}$-octadecane at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{array}{lll}
\log P=A-B /(T / K) & (1) & \ln P=A-B /(T / K) \\
\log P=A-B /\left(C+t /{ }^{\circ} C\right) & (2) & \ln P=A-B /\left(C+t /{ }^{\circ} C\right) \\
\log P=A-B /(C+T / K) & (3) & \\
\log P=A-B /(T / K)-C \cdot \log (T / K) & (4) & \\
\ln \left(P / P_{\text {ref }}\right)=\left[1-\left(T_{\text {ref }} / T\right)\right] \cdot \exp \left(a+b T+c T^{2}\right) & (5)-C o x \text { eq. } &
\end{array}
$$

1. 

| Stull 1947 |  | Myers \& Fenske 1955 |  | Zwolinski \& Wilhoit 1971 |  | Macknick \& Prausnitz 1979 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 119.6 | 133.3 | 102.4 | 26.66 | 172.3 | 1333 | 45.0 | 0.220 |
| 152.1 | 666.6 | 115.9 | 66.66 | 189.0 | 2666 | 51.45 | 0.400 |
| 169.6 | 1333 | 127.0 | 133.3 | 199.6 | 4000 | 54.5 | 0.568 |
| 187.5 | 2666 | 139.6 | 266.6 | 207.5 | 5333 | 54.85 | 0.591 |
| 207.4 | 5333 | 147.0 | 400.0 | 213.9 | 6666 | 59.85 | 0.935 |
| 219.7 | 7999 | 153.3 | 533.3 | 219.3 | 7999 | 65.60 | 1.529 |
| 236.0 | 13332 | 157.7 | 666.6 | 228.2 | 10666 | 71.25 | 2.493 |
| 260.6 | 26664 | 161.8 | 799.9 | 234.39 | 13332 | 80.85 | 5.826 |
| 288.0 | 53329 | 167.7 | 1067 | 249.21 | 19998 | 84.10 | 7.148 |
| 317.0 | 101325 | 172.8 | 1333 | 259.64 | 26664 | 88.10 | 9.719 |
|  |  | 182.8 | 2000 | 268.12 | 33331 |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 28 | 189.6 | 2666 | 275.32 | 39997 | eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | 199.9 | 4000 | 287.2 | 53329 | A | 25.548 |
|  |  | 208.0 | 5333 | 296.9 | 66661 | B | 10165 |
|  |  | 214.3 | 6666 | 305.2 | 79993 |  |  |
|  |  | 219.5 | 7999 | 312.4 | 93326 |  |  |
|  |  | 228.5 | 10666 | 313.7 | 95992 |  |  |
|  |  | 235.7 | 13332 | 315.0 | 98659 |  |  |
|  |  | 249.0 | 19998 | 316.3 | 101325 |  |  |
|  |  | 259.2 | 26664 |  |  |  |  |
|  |  | 273.8 | 39997 | bp/ ${ }^{\circ} \mathrm{C}$ | 316.3 |  |  |
|  |  | 286.0 | 53329 |  |  |  |  |
|  |  | 294.7 | 66661 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  | 302 | 79993 | A | 7.0022 |  |  |
|  |  | 308 | 93326 | B | 1894.3 |  |  |
|  |  | 313 | 101325 | C | 143.30 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ | $\left.{ }^{1}\right)=$ |  |  |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 90.8 |  |  |
|  |  |  |  | at bp | 54.48 |  |  |

TABLE 2.1.1.1.34.1 (Continued)
2.

| Allemand et al. 1986 |  | Morgan \& Kobayashi 1994 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation |  | vapor-liquid equilibrium |  | recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathrm{P} / \mathrm{Pa}$ |
| 62.04 | 1.1506 | 139.919 | 256.6 | 311.88 | 0.1 |
| 71.39 | 2.680 | 149.924 | 443.6 | 334.61 | 1.0 |
| 84.0 | 6.599 | 159.93 | 729.4 | 362.08 | 10 |
| 88.0 | 9.479 | 169.936 | 1148 | 396.24 | 100 |
| 97.0 | 18.40 | 179.974 | 1761 | 440.41 | 1000 |
| 100.4 | 22.00 | 189.948 | 2637 | 500.70 | 10000 |
| 110.0 | 43.86 | 199.976 | 3870 | 590.02 | 101325 |
| 124.21 | 106.1 | 209.976 | 5566 | 298.15 | 0.02007 |
| 130.0 | 152.0 | 219.976 | 7834 |  |  |
| 140.0 | 264.0 | 229.977 | 10835 | Cox eq. |  |
| 166.67 | 995.9 | 239.970 | 14744 | $\text { eq. } 5$ | P/kPa |
|  |  | 254.979 | 22736 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
|  |  | 254.979 | 27300 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 469.64 |
|  |  | 264.979 | 34026 | a | 3.24741 |
|  |  | 284.980 | 49559 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.048039 |
|  |  | 299.98 | 70490 | $10^{6} \mathrm{c} / \mathrm{K}^{-2}$ | 1.362445 |
|  |  | 314.982 | 98240 |  |  |
|  |  | data fitted | gner eq. |  |  |



FIGURE 2.1.1.1.34.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-octadecane.

### 2.1.1.1.35

n-Eicosane


Common Name: Eicosane
Synonym: didecyl
Chemical Name: $n$-eicosane
CAS Registry No: 112-95-8
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{42} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{18} \mathrm{CH}_{3}$
Molecular Weight: 282.547
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): 36.6 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : $334.8 \quad$ (Chirico et al. 1989)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
0.7887, $0.7853 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
0.7886 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
451.4 (calculated-Le Bas molar volume at normal boiling point)
$358.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
358 (Wang et al. 1992)
Enthalpy of vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
63.93; 64.35 (exptl., calculated, Macknick \& Prausnitz 1979b)
100.9; $110 \quad\left(25,94^{\circ} \mathrm{C}\right.$, Piacente et al. 1994)
$101.81 \quad$ (298.15 K, recommended, Ruzicka \& Majer 1994)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
69.875 (Dreisbach 1959)
69.5 (Piacente et al. 1994)
67.8 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
219.6, 203.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.769\left(\mathrm{mp}\right.$ at $36.6^{\circ} \mathrm{C}$ )

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
$1.9 \times 10^{-3}, 8.0 \times 10^{-4}$ (shake flask-GC, distilled water; seawater, Sutton \& Calder 1974) $1.10 \times 10^{-7}$ (extrapolated from data of McAuliffe 1966, Coates et al. 1985) $3.11 \times 10^{-7}$ (extrapolated from data of McAuliffe 1966, Eastcott et al. 1985)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$13.33^{*} \quad\left(121.9^{\circ} \mathrm{C}\right.$, static method -Hg manometer, measured range $121.9-342.0^{\circ} \mathrm{C}$, Myers \& Fenske 1955) $\log (\mathrm{P} / \mathrm{mmHg})=7.0225-1948.7 /\left(127.8+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range: $224-417^{\circ} \mathrm{C}$, (Antoine eq. for liquid state, Dreisbach 1959)
$1333^{*} \quad\left(198.3^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $198.3-343.8^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.1522-2032.7 /\left(132.1+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $198.3-379^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
0.41* $\quad\left(71.5^{\circ} \mathrm{C}, \mathrm{P}_{\mathrm{L}}\right.$, gas saturation-IR, Macknick \& Prausnitz 1979)
$\ln \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=26.849-11230 /(\mathrm{T} / \mathrm{K})$; temp range: $71.15-107.3^{\circ} \mathrm{C}$, (Antoine eq., gas saturation, liquid state, Macknick \& Prausnitz 1979)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=10.77373-4872.63 /(\mathrm{T} / \mathrm{K})$; temp range: $344-380 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.2771-2032.7 /(\mathrm{T} / \mathrm{K}-141.05)$; temp range $528-620 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$0.201^{*} \quad\left(79.97^{\circ} \mathrm{C}\right.$, pressure gauge, measured range $90.07-194.21^{\circ} \mathrm{C}$, Sasse et al. 1988)
$\log (\mathrm{P} / \mathrm{mmHg})=7.95834-2665.762 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+167.047\right)$; (Antoine eq. derived from exptl. data, liquid phase, pressure gauge measurement, Sasse et al. 1988)
15.6* $\quad\left(115^{\circ} \mathrm{C}\right.$, inclined piston measurement, temp range $115-215^{\circ} \mathrm{C}$, Chirico et al. 1989)
$\ln (\mathrm{P} / \mathrm{kPa})=19.36-9083 /(\mathrm{T} / \mathrm{K})$; temp range $406-472 \mathrm{~K}$ (transpiration method, Piacente et al. 1991)
$\ln (\mathrm{P} / \mathrm{kPa})=22.53-10649 /(\mathrm{T} / \mathrm{K})$; temp range $345-393 \mathrm{~K}$ (torsion method, Piacente et al. 1991)
$\ln (\mathrm{P} / \mathrm{kPa})=18.10-7889 /[(\mathrm{T} / \mathrm{K})+32]$; temp range $315-472 \mathrm{~K}$ (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)
$\log (\mathrm{P} / \mathrm{mmHg})=7.1522-2032.1 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+132.10\right)$; temp range $198-379^{\circ} \mathrm{C}$ (Antoine eq., Dean 1992)
$0.32^{*}, 0.641\left(74,78^{\circ} \mathrm{C}\right.$, torsion-effusion method, measured range $74-115^{\circ} \mathrm{C}$, Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.37-5785 /(\mathrm{T} / \mathrm{K})$; temp range $351-384 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=12.96-5709 /(\mathrm{T} / \mathrm{K})$; temp range $347-389 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.16-5747 /(\mathrm{T} / \mathrm{K})$; temp range $\sim 347-388 \mathrm{~K}, \Delta \mathrm{H}_{\mathrm{V}}=110 \mathrm{~kJ} \mathrm{~mol}^{-1}$ (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)
0.002091* (recommended, Ruzicka \& Majer 1994)
$\ln \left[(\mathrm{P} / \mathrm{kPa}) /\left(\mathrm{P}_{\mathrm{o}} / \mathrm{kPa}\right)\right]=\left[1-\left(\mathrm{T}_{\mathrm{o}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right] \cdot \exp \left\{3.31181-2.102218 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.348780 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; reference state at $\mathrm{P}_{\mathrm{o}}=101.325 \mathrm{kPa}, \mathrm{T}_{\mathrm{o}}=617.415 \mathrm{~K}$ (Cox equation, Ruzicka \& Majer 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=19.4193-5.8699 \times 10^{3} /(\mathrm{T} / \mathrm{K})-44.282 \cdot \log (\mathrm{~T} / \mathrm{K})-1.2606 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+5.2241 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $310-767 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
0.00209* (GC-retention time correlation, Chickos \& Hanshaw 2004)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
198300 (calculated-P/C, Eastcott et al. 1988)
32.73 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
10.39 (HPLC-k' correlation, Coates et al. 1985)
10.0; 8.92 (calculated-fragment const.; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<31 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993)
Half-Lives in the Environment:

TABLE 2.1.1.1.35.1
Reported vapor pressures of eicosane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp (\mathrm{a}+\mathrm{bT}+\mathrm{cT})^{2}$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
(2) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(3)
(3a)
(4)
1.

| Myers \& Fenske 1955 |  | Zwolinski \& Wilhoit 1971 |  | Macknick \& Prausnitz 1979 |  | Sasse et al. 1988 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Hg manometer |  | selected values |  | gas saturation |  | electronic manometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 121.9 | 13.33 | 198.3 | 1333 | 71.15 | 0.4106 | 90.07 | 2.333 |
| 136.5 | 66.6 | 215.3 | 2666 | 79.90 | 0.973 | 90.12 | 2.360 |
| 148.6 | 133.3 | 326.1 | 4000 | 86.70 | 1.693 | 100.17 | 5.526 |
| 162.0 | 266.6 | 234.1 | 5333 | 90.35 | 2.333 | 100.17 | 5.266 |
| 170.0 | 400.0 | 240.7 | 6666 | 94.50 | 3.266 | 110.16 | 11.49 |
| 176.7 | 533.3 | 246.1 | 7999 | 102.95 | 6.719 | 110.16 | 11.43 |
| 182.0 | 666.6 | 255.15 | 10666 | 107.30 | 9.133 | 120.06 | 22.53 |
| 185.7 | 799.9 | 262.41 | 13332 |  |  | 120.10 | 22.80 |
| 192.6 | 1067 | 276.39 | 19998 |  |  | 130.11 | 43.20 |
| 198.0 | 1333 | 286.91 | 26664 | eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ | 130.13 | 43.73 |
| 208.8 | 2000 | 295.45 | 33331 | A | 26.849 | 139.99 | 80.66 |
| 215.7 | 2666 | 302.70 | 39997 | B | 11230 | 140.03 | 79.86 |
| 226.4 | 4000 | 314.60 | 53329 |  |  | 149.88 | 141.61 |
| 234.7 | 5333 | 324.4 | 66661 |  |  | 149.97 | 144.9 |
| 241.3 | 6666 | 332.6 | 79993 |  |  | 159.73 | 243.7 |
| 246.5 | 7999 | 339.8 | 93326 |  |  | 159.83 | 245.7 |
| 255.7 | 10666 | 341.2 | 95992 |  |  | 169.61 | 404.2 |
| 262.5 | 13332 | 342.5 | 98659 |  |  | 169.68 | 410.6 |
| 276.1 | 19998 | 343.8 | 101325 |  |  | 179.49 | 657.3 |
| 286.4 | 26664 |  |  |  |  | 189.25 | 1025 |
| 300.2 | 39997 | bp/ ${ }^{\circ} \mathrm{C}$ | 343.8 |  |  | 194.21 | 1266 |
| 312.0 | 53329 |  |  |  |  |  |  |
| 320.0 | 66661 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 327.0 | 79993 | A | 7.1522 |  |  | A | 7.99897 |
| 333.0 | 93326 | B | 2032.7 |  |  | B | 2067.622 |
| 342.0 | 101325 | C | 132.1 |  |  | C | 177.32 |
|  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  |  |  |
|  |  | at $25^{\circ} \mathrm{C}$ | 100.8 |  |  |  |  |
|  |  |  | 57.49 |  |  |  |  |

TABLE 2.1.1.1.35.1 (Continued)
2.

Chirico et al. 1989

(Continued)

TABLE 2.1.1.1.35.1 (Continued)
3.

Piacente et al. 1991 (cont'd)


## TABLE 2.1.1.1.35.1 (Continued)

4. 

| Piacente et al. 1994 |  |  |  | Morgan \& Kobayashi 1994 |  | Ruzicka \& Majer 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| torsion-effusion |  |  |  | static pressure gauge |  | recommended |  |
| $t^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| run a |  | run b |  | top-cut |  |  |  |
| 77.85 | 0.641 | 73.85 | 0.32 | 159.903 | 244 | 330.01 | 0.1 |
| 79.85 | 0.961 | 77.85 | 0.481 | 169.91 | 401.8 | 353.55 | 1.0 |
| 81.85 | 1.28 | 80.85 | 0.641 | 179.918 | 641.1 | 381.97 | 10 |
| 83.85 | 1.52 | 82.85 | 0.801 | 189.926 | 1006 | 417.30 | 100 |
| 85.85 | 1.84 | 85.85 | 1.28 | 199.934 | 1537 | 462.95 | 1000 |
| 88.85 | 2.40 | 88.85 | 1.60 | 199.976 | 1538 | 525.23 | 10000 |
| 91.85 | 3.36 | 91.85 | 2.40 | 209.976 | 2301 | 617.41 | 101325 |
| 93.85 | 4.17 | 94.85 | 3.04 | 219.947 | 3358 | 298.15 | 0.002091 |
| 94.85 | 4.97 | 97.85 | 4.17 | 229.954 | 4812 |  |  |
| 98.85 | 6.57 | 100.85 | 4.65 | 239.961 | 6771 | Coxeq. |  |
| 101.85 | 8.33 | 103.85 | 6.89 | 249.969 | 9359 | eq. 5 | P/kPa |
| 103.85 | 10.40 | 106.85 | 8.65 | 259.979 | 12738 | $\mathrm{P}_{\text {ref }} / \mathrm{kPa}$ | 101.325 |
| 107.85 | 15.1 | 112.85 | 14.3 | 269.979 | 17040 | $\mathrm{T}_{\text {ref }} / \mathrm{K}$ | 617.415 |
| 110.85 | 19.4 | 114.85 | 17.1 | 284.980 | 25728 | a | 3.31181 |
|  |  |  |  | 299.980 | 37745 | $10^{3} \mathrm{~b} / \mathrm{K}^{-1}$ | -2.102218 |
| eq. for run a |  | eq. for ru |  | 314.982 | 54210 | $10^{6} / \mathrm{K}^{-2}$ | 1.248780 |
| eq. 1 | $\mathrm{P} / \mathrm{kPa}$ | eq. 1 | P/kPa | mid-cut |  |  |  |
| A | 13.37 | A | 12.96 | 159.847 | 244.9 |  |  |
| B | 5785 | B | 5709 | 169.853 | 401 |  |  |
| temp range: $351-384 \mathrm{~K}$ |  | temp range: $347-388 \mathrm{~K}$ |  | 179.860 | 639 |  |  |
|  |  | 189.875 | 999.1 |  |  |
| $\begin{aligned} & \left.\Delta \mathrm{H}_{\mathrm{V}} / \mathrm{kJ} \mathrm{~mol}^{-1}\right)= \\ & \text { at } 298.15 \mathrm{~K} \\ & \text { at } 367 \mathrm{~K} \end{aligned}$ |  |  |  | By weighing the slopes and intercepts of above 2 eq., selected vapor pressure eq. |  | 199.874 | 1541 |  |  |
|  | 100.9 | 209.884 | 2302 |  |  |  |  |
|  | $110 \pm 2$ | 219.894 | 3349 |  |  |  |  |
|  |  | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ | 229.911 | 4813 |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 28 | A | 13.16 | 239.915 | 6773 |  |  |
| $\Delta \mathrm{H}_{\mathrm{fus}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=61.10$ |  | B $\quad 5747$ |  | 249.931 | 9349 |  |  |
|  |  | 259.938 | 12736 |  |  |
| $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)$ | $152.7$ |  |  | $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{v}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=110 \pm 2 \\ & \text { at } 367 \mathrm{~K} \end{aligned}$ |  | 269.949 | 17029 |  |  |
|  |  | 279.957 | 22549 |  |  |  |  |
|  |  | 289.970 | 29252 |  |  |  |  |
|  |  | 299.970 | 37754 |  |  |  |  |
|  |  | 309.982 | 48080 |  |  |  |  |
|  |  | data fitted to Wagner eq. |  |  |  |  |  |



FIGURE 2.1.1.1.35.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-eicosane.

### 2.1.1.1.36 <br> n-Tetracosane



Common Name: Tetracosane
Synonym:
Chemical Name: $n$-tetracosane
CAS Registry No: 646-31-1
Molecular Formula: $\mathrm{C}_{24} \mathrm{H}_{50} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{22} \mathrm{CH}_{3}$
Molecular Weight: 338.654
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
50.4 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
391.3 (Dreisbach 1959; Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.7991,0.7958\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
540.2 (calculated-Le Bas method at normal boiling point)
$423.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
Enthalpy of vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$126 \quad\left(132^{\circ} \mathrm{C}\right.$, Piacente et al. 1994)
121.9 (calculated, Chickos \& Hanshaw 2004)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$54.9 \quad$ (Dreisbach 1959; Piacente et al. 1994)
31.3, 54.89; 86.19 (48.15, $50.95^{\circ} \mathrm{C}$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
266.79, 240.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.563\left(\mathrm{mp}\right.$ at $50.4^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ : $5.8 \times 10^{-10}$ (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$133.3^{*} \quad\left(183.8^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $183.8-386.4^{\circ} \mathrm{C}$, Stull 1947$)$
$\log (\mathrm{P} / \mathrm{mmHg})=7.53923-2591.9 /\left(165.1+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $260-500^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0976-2112.0 /\left(109.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ (Antoine eq., Kudchadker \& Zwolinski 1966)
66.66* $\quad\left(175.9^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $175.9-391.3^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0976-2112.0 /\left(109.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $175.9-391.3^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 19642.5 /(\mathrm{T} / \mathrm{K})]+9.408166$; temp range $183.8-386.4^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.44051-2289.02 /(\mathrm{T} / \mathrm{K}-147.92)$; temp range $498-573 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$0.253^{*} \quad\left(100.26^{\circ} \mathrm{C}\right.$, pressure gauge, Sasse et al. 1988)
$\log (\mathrm{P} / \mathrm{mmHg})=7.17666-2243.665 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+126.236\right)$; temp range $100.26-149.23^{\circ} \mathrm{C}$ (Antoine eq. derived from exptl. data, liquid phase, Sasse et al. 1988)
$\log (\mathrm{P} / \mathrm{kPa})=(8.76 \pm 0.50)-(4501 \pm 250) /(\mathrm{T} / \mathrm{K})$; temp range $451-497 \mathrm{~K}$ (Antoine eq. from exptl. data, transpiration method, Piacente \& Scardala 1990; quoted, Pompili \& Piacente 1990)
$\ln (\mathrm{P} / \mathrm{kPa})=21.25-10946 /(\mathrm{T} / \mathrm{K})$; temp range $501-523 \mathrm{~K}$ (transpiration method, Piacente et al. 1991)
$\ln (\mathrm{P} / \mathrm{kPa})=25.35-12399 /(\mathrm{T} / \mathrm{K})$; temp range $376-438 \mathrm{~K}$ (torsion method, Piacente et al. 1991)
$\ln (\mathrm{P} / \mathrm{kPa})=18.38-8349 /[(\mathrm{T} / \mathrm{K})+58]$; temp range $343-523 \mathrm{~K}$ (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)
$90.1^{*} \quad\left(179.916^{\circ} \mathrm{C}\right.$, static-differential pressure, measured range $179.916-314.820^{\circ} \mathrm{C}$, Morgan \& Kobayashi 1994)
$0.721^{*}, 0.801\left(114,115^{\circ} \mathrm{C}\right.$, torsion-effusion, measured range 386-425 K, Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.57-6459 /(\mathrm{T} / \mathrm{K})$; temp range $388-413 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=14.25-6726 /(\mathrm{T} / \mathrm{K})$; temp range $387-423 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.92-6591 /(\mathrm{T} / \mathrm{K})$; temp range $386-425 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.96-6608 /(\mathrm{T} / \mathrm{K})$; temp range $\sim 386-425 \mathrm{~K}, \Delta \mathrm{H}_{\mathrm{V}}=126 \mathrm{~kJ} \mathrm{~mol}^{-1}$ (selected Antoine eq. based
on exptl. data, torsion-effusion method, Piacente et al. 1994)
$3.30 \times 10^{-5}$ (quoted from Daubert \& Danner 1997, Goss \& Schwarzenbach 1999)
$2.37 \times 10^{-5} \quad$ (GC-retention time correlation, Chickos \& Hanshaw 2004)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
12.53 (HPLC-k' correlation, Coates et al. 1985)
12.0; 10.5 (calculated-fragment const; calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<31 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993)
Half-Lives in the Environment:

## TABLE 2.1.1.1.36.1

Reported vapor pressures of tetracosane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{t} / \mathrm{K})$ |

1. 

| Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  | Sasse et al. 1988 |  | Piacente et al. 1990 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | selected values |  | electronic manometry |  | transpiration |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
|  |  |  |  |  |  | run A |  |
| 183.8 | 133.3 | 175.9 | 66.66 | 100.26 | 0.255 | 183.85 | 85.11 |
| 219.6 | 666.6 | 188.0 | 133.3 | 110.25 | 0.613 | 185.85 | 100.0 |
| 237.6 | 1333 | 201.1 | 266.6 | 120.21 | 1.560 | 187.85 | 97.72 |
| 255.3 | 2666 | 220.5 | 666.6 | 130.15 | 3.506 | 189.85 | 107.2 |
| 276.3 | 5333 | 236.8 | 1333 | 139.93 | 7.386 | 193.85 | 134.9 |
| 288.4 | 7999 | 391.3 | 101325 | 140.09 | 7.506 | 195.85 | 151.4 |
| 305.2 | 13332 |  |  | 149.92 | 14.80 | For run A:- |  |
| 330.3 | 66661 | bp/ ${ }^{\circ} \mathrm{C}$ | 391.3 | 149.97 | 14.80 | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ |
| 358.0 | 53329 |  |  | 159.77 | 28.53 | A | 8.17 |
| 386.4 | 101325 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 159.62 | 52.13 | B | 4221 |
|  |  | A | 7.0976 | 179.45 | 91.06 | For temp ran | 57-469 K |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 51.1 | B | 2112.0 | 189.23 | 148.9 | Run B |  |

TABLE 2.1.1.1.36.1 (Continued)

| Stull 1947 | Zwolinski \& Wilhoit 1971 |  | Sasse et al. 1988 |  | Piacente et al. 1990 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data | selected values |  | electronic manometry |  | transpiration |  |
| $\mathbf{t}{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  | C | 109.6 |  |  | 187.85 | 104.7 |
|  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 192.85 | 138.0 |
|  |  |  | A | 7.16777 | 197.85 | 182.0 |
|  |  |  | B | 2243.665 | 206.85 | 288.4 |
|  |  |  | C | 126.336 | 209.85 | 295.1 |
|  |  |  |  |  | 212.35 | 316.2 |
|  |  |  |  |  | 215.85 | 426.6 |
|  |  |  |  |  | 216.85 | 436.5 |
|  |  |  |  |  | 217.35 | 446.7 |
|  |  |  |  |  | 217.88 | 457.1 |
|  |  |  |  |  | 222.35 | 588.8 |
|  |  |  |  |  | 223.35 | 616.6 |
|  |  |  |  |  | for run B:- |  |
|  |  |  |  |  | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ |
|  |  |  |  |  | A | 9.53 |
|  |  |  |  |  | B | 4843 |
|  |  |  |  |  | for temp r | 61-496 K |

2. 

Piacente et al. 1990 (cont'd)
Piacente et al. 1991

| transpiration method |  | transpiration method |  | torsion method |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | $t /{ }^{\circ} \mathrm{C}$ | P/Pa |
| run C |  |  |  | cell B |  | cont'd |  |
| 177.85 | 61.66 | 227.85 | 537.0 | 109.05 | 0.955 | 136.85 | 9.772 |
| 184.85 | 79.43 | 230.85 | 602.6 | 118.35 | 1.514 | 138.85 | 11.22 |
| 187.85 | 85.11 | 234.85 | 741.3 | 122.35 | 2.089 | 141.85 | 13.49 |
| 189.85 | 97.72 | 238.85 | 871.0 | 126.35 | 2.291 | 142.85 | 14.79 |
| 192.35 | 102.3 | 240.85 | 933.3 | 129.35 | 3.020 | 144.85 | 15.85 |
| 193.85 | 117.5 | 242.85 | 1096 | 131.35 | 3.388 | 147.85 | 19.05 |
| 194.85 | 141.25 | 245.85 | 1175 | 134.35 | 4.365 | 148.85 | 21.38 |
| 196.85 | 123.0 | 246.85 | 1259 | 136.35 | 4.898 | 149.85 | 23.44 |
| 201.35 | 141.25 | 247.85 | 1047 | 138.35 | 6.457 | 152.35 | 26.30 |
| 205.85 | 199.5 | 249.85 | 1148 | 141.35 | 7.943 | 154.85 | 29.51 |
| 209.85 | 245.5 |  |  | 143.35 | 10.23 | 158.85 | 39.81 |
| 212.85 | 288.4 | For tra | ration data: | 145.35 | 11.75 | 160.35 | 44.67 |
| 213.85 | 302.0 | eq. 1a | P/kPa | 147.35 | 13.80 | 162.35 | 51.29 |
|  |  | A | $21.25 \pm 1.08$ | cell D |  | cell D |  |
|  |  | B | $10946 \pm 554$ | 123.85 | 2.951 | 126.85 | 2.344 |
| for transpiration data: |  |  |  | 126.85 | 3.981 | 130.85 | 3.548 |
| eq. 1 | $\mathrm{P} / \mathrm{kPa}$ |  |  | 129.85 | 4.677 | 134.8513885 | 4.577 |
| A | $8.31 \pm 1.08$ |  |  | 133.85 | 5.888 | 139.85 | 5.888 |
| B | $4314 \pm 211$ |  |  | 135.85 | 7.079 | 140.85 | 6.457 |
| for temp range: 451-487 K |  |  |  | 137.85 | 8.128 | 142.85 | 9.333 |
|  |  |  |  | 139.85 | 8.128 | 144.85 | 10.47 |
| overall | essure eq. by |  |  | 142.85 | 9.333 | 147.85 | 12.88 |

TABLE 2.1.1.1.36.1 (Continued)
Piacente et al. 1990 (cont'd)
Piacente et al. 1991

| transpiration method |  | transpiration method |  | torsion method |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| weighted slopes and intercepts |  |  |  | 145.85 | 14.125 | 149.85 | 15.14 |
| eq. 1 | $\mathrm{P} / \mathrm{kPa}$ |  |  | 148.85 | 18.20 | 152.85 | 17.78 |
| A | $8.76 \pm 0.50$ |  |  | 151.85 | 36.31 | 153.85 | 18.62 |
|  | $4501 \pm 250$ |  |  | cell A |  | 156.85 | 22.39 |
|  |  |  |  | 102.85 | 0.7413 | 162.85 | 33.11 |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=86 \pm 5 \\ & \text { at } 474 \mathrm{~K} \end{aligned}$ |  |  |  | 104.85 | 0.8511 | 164.85 | 36.31 |
|  |  |  |  | 106.95 | 0.9772 |  |  |
|  |  |  |  | 109.85 | 1.2303 | for torsion method data:- |  |
|  |  |  |  | 114.85 | 1.5849 | eq. 1a | $\mathrm{P} / \mathrm{kPa}$ |
|  |  |  |  | 118.85 | 2.344 | A | $25.35 \pm 0.60$ |
|  |  |  |  | 126.85 | 4.169 | B | $12399 \pm 575$ |
|  |  |  |  | 127.85 | 4.898 |  |  |
|  |  |  |  | 129.85 | 5.623 |  |  |
|  |  |  |  | 131.85 | 6.918 |  |  |
|  |  |  |  | 133.85 | 8.128 |  |  |

3. 

Piacente et al. 1991 (cont'd)
Piacente et al. 1994


## TABLE 2.1.1.1.36.1 (Continued)

Piacente et al. 1991 (cont'd)
Piacente et al. 1994

| Knudsen effusion |  | torsion-effusion |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 209.939 | 415.6 |  |  |  |  |  |  |
| 219.946 | 652.9 |  |  | $\mathrm{mp} / \mathrm{K}$ | 322 |  |  |
| 229.950 | 1001 |  |  | $\Delta \mathrm{H}_{\text {fus }} /(\mathrm{kJ}$ | 54.9 |  |  |
| 239.960 | 1506 |  |  | $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ}$ | 180.9 |  |  |
| 249.971 | 2209 |  |  | at 298.15 |  |  |  |
| 259.979 | 3176 |  |  |  |  |  |  |
| 260.979 | 4489 |  |  |  |  |  |  |
| 284.980 | 7303 |  |  |  |  |  |  |
| 299.980 | 11470 |  |  |  |  |  |  |
| 314.820 | 17460 |  |  |  |  |  |  |



FIGURE 2.1.1.1.36.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-tetracosane.

### 2.1.1.1.37 $n$-Hexacosane



Common Name: Hexacosane
Synonym: cerane
Chemical Name: n-hexacosane
CAS Registry No: 631-01-3
Molecular Formula: $\mathrm{C}_{26} \mathrm{H}_{54} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{24} \mathrm{CH}_{3}$
Molecular Weight: 366.707
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
56.1 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
412.2 (Dreisbach 1959; Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.8032,0.7998 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
$0.8032 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
584.6 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
$456.6 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
457 (Wang et al. 1992)
Enthalpy of vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
64.806 (bp, Dreisbach 1959)
131.2 (calculated, Chickos \& Hanshaw 2004)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
32.3, 59.5; $95.3 \quad\left(53.35,56.35^{\circ} \mathrm{C}\right.$, total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
289.03, 259.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ): $\mathrm{F}: 0.495\left(\mathrm{mp}\right.$ at $56.1^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
$1.7 \times 10^{-3} ; 1.0 \times 10^{-4}$ (shake flask-GC, distilled water; seawater, Sutton \& Calder 1974)
$1.33 \times 10^{-10} \quad($ extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$133.3^{*} \quad\left(204.0^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $204.0-399.8^{\circ} \mathrm{C}$, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=7.57689-2692.73 /\left(161.2+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $278-500^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=7.1096-2164.3 /\left(99.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ (Antoine eq., Kudchadker \& Zwolinski 1966)
66.66* $\quad\left(192.5^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $192.5-412.2^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.1096-2164.3 /\left(99.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $192.6-412.2^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 21605.7 /(\mathrm{T} / \mathrm{K})]+9.899820$; temp range $204-399.8^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.2345-2164.3 /(\mathrm{T} / \mathrm{K}-173.55)$; temp range $466-685 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=9.44384-4935.969 /(\mathrm{T} / \mathrm{K})$; temp range $478-530 \mathrm{~K}$ (Antoine eq., liquid, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{kPa})=(9.93 \pm 0.50)-(5168 \pm 200) /(\mathrm{T} / \mathrm{K})$; temp range $455-519 \mathrm{~K}$, (Antoine eq. from exptl. data, transpiration, Piacente \& Scardala 1990; Pompili \& Piacente 1990)
$\ln (\mathrm{P} / \mathrm{kPa})=18.63-9892 /(\mathrm{T} / \mathrm{K})$; temp range $506-546 \mathrm{~K}$ (transpiration method, Piacente et al. 1991)
$\ln (\mathrm{P} / \mathrm{kPa})=28.91-14285 /(\mathrm{T} / \mathrm{K})$; temp range $391-442 \mathrm{~K}$ (torsion method, Piacente et al. 1991)
$\ln (\mathrm{P} / \mathrm{kPa})=17.76-8050 /[(\mathrm{T} / \mathrm{K})+72]$; temp range $356-546 \mathrm{~K}$ (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)
$\log (\mathrm{P} / \mathrm{kPa})=14.50-7084 /(\mathrm{T} / \mathrm{K})$; temp range $420-437 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.75-6765 /(\mathrm{T} / \mathrm{K})$; temp range $391-433 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=13.65-6748 /(\mathrm{T} / \mathrm{K})$; temp range $392-431 \mathrm{~K}$ (torsion-effusion, Antoine eq., Piacente et al. 1994)
$\log (\mathrm{P} / \mathrm{kPa})=14.01-6682 /(\mathrm{T} / \mathrm{K})$; temp range $\sim 392-437 \mathrm{~K}, \Delta \mathrm{H}_{\mathrm{V}}=132 \mathrm{~kJ} \mathrm{~mol}^{-1}$ (selected Antoine eq. based
on exptl. data, torsion-effusion method, Piacente et al. 1994)
$5.03 \times 10^{-6}$ (quoted from Daubert \& Danner 1997, Goss \& Schwarzenbach 1999)
$2.82 \times 10^{-6}($ GC-retention time correlation, Chickos \& Hanshaw 2004)
Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
21200 (calculated-P/C, Eastcott et al. 1988)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
13.0, 11.4 (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Biodegradation: microbial degradation $\mathrm{t}_{1 / 2}<31 \mathrm{~d}$ by Pseudomonas sp. (Setti et al. 1993)
Half-Lives in the Environment:

TABLE 2.1.1.1.37.1
Reported vapor pressures of hexacosane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K}$

$$
\begin{align*}
& \log P=A-B /(C+C / K)-C \cdot \log (T / K)  \tag{2}\\
& \log P=A-B /(T / K)
\end{align*}
$$

1. 

| Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  | Piacente et al. 1990 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | selected values |  | transpiration |  | transpiration (continued) |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  |  |  | run A |  | run C |  |
| 204.0 | 133.3 | 192.5 | 66.66 | 187.85 | 64.57 | 182.35 | 37.15 |
| 240.0 | 666.6 | 204.8 | 133.3 | 194.35 | 74.13 | 188.85 | 54.95 |
| 257.4 | 1333 | 218.3 | 266.6 | 197.35 | 91.20 | 193.35 | 70.79 |
| 275.8 | 2666 | 138.0 | 666.6 | 197.85 | 100.0 | 196.85 | 89.13 |
| 295.2 | 5333 | 254.6 | 527.75 | 198.35 | 97.72 | 199.85 | 104.7 |
| 307.8 | 7999 | 412.2 | 101325 | 199.85 | 109.65 | 202.35 | 123.0 |
| 323.2 | 13332 |  |  | 202.85 | 129.8 | 203.85 | 131.8 |
| 348.4 | 66661 |  |  | 205.85 | 131.8 | 204.85 | 112.2 |
| 374.5 | 53329 | bp/ ${ }^{\circ} \mathrm{C}$ | 412.2 | 208.85 | 162.2 | 206.85 | 134.9 |
| 399.8 | 101325 |  |  | 211.85 | 251.2 | 210.85 | 229.1 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 214.85 | 263.0 | 215.35 | 288.4 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 56.6 | A | 7.1096 | eq. for run $\mathrm{A}:-$ |  | 218.85 | 263.0 |
|  |  | B | 2164.3 | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ | 221.85 | 309.0 |
|  |  | C | 99.6 | A | $10.40 \pm 0.42$ | 223.35 | 346.7 |

TABLE 2.1.1.1.37.1 (Continued)

2.

Piacente et al. 1991

| transpiration method |  | torsion method |  | torsion (continued) |  | torsion (continued) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  | cell E |  | cell A |  | cell B |  |
| 232.85 | 354.8 | 131.35 | 1.202 | 141.35 | 1.479 | 138.85 | 3.020 |
| 238.35 | 616.6 | 132.35 | 1.380 | 143.35 | 1.950 | 142.85 | 4.571 |
| 242.85 | 616.6 | 134.35 | 1.585 | 145.35 | 2.692 | 144.85 | 4.169 |
| 242.85 | 616.6 | 136.35 | 1.778 | 146.35 | 3.162 | 144.85 | 4.898 |
| 246.35 | 575.4 | 137.35 | 1.995 | 146.85 | 3.715 | 147.35 | 6.166 |
| 247.85 | 660.7 | 139.35 | 2.570 | 147.35 | 4.169 | 150.35 | 6.457 |
| 249.35 | 758.6 | 140.85 | 3.020 | 147.85 | 4.898 | 153.85 | 9.550 |
| 251.35 | 871.0 | 142.35 | 3.388 | 148.35 | 5.623 | 154.35 | 9.120 |
| 252.35 | 933.3 | 146.35 | 5.129 | 148.85 | 6.310 | 154.35 | 9.550 |
| 254.35 | 933.3 | 148.35 | 6.166 | 149.35 | 7.586 | 154.85 | 9.550 |
| 255.85 | 1023 | 150.35 | 6.918 | 150.35 | 9.120 | 155.85 | 10.72 |
| 256.35 | 871.0 | 153.35 | 7.762 | 152.35 | 10.47 | 155.85 | 10.96 |
| 258.85 | 1047 | 155.35 | 9.120 | 154.35 | 11.22 | 158.85 | 13.80 |
| 259.35 | 1148 | 158.35 | 12.30 | 165.35 | 12.88 | cell A |  |
| 261.85 | 1288 | 160.35 | 14.13 | 158.35 | 15.49 | 132.85 | 2.455 |
| 262.85 | 1288 | 163.35 | 17.38 | 160.35 | 18.62 | 135.35 | 2.951 |
| 266.35 | 1230 | 165.35 | 20.42 | cell A |  | 138.85 | 3.890 |
| 266.35 | 1259 | 167.35 | 23.99 | 117.85 | 0.490 | 142.35 | 5.129 |
| 268.35 | 1445 | 169.35 | 28.18 | 123.85 | 0.741 | 143.85 | 5.623 |
| 269.35 | 1413 |  |  | 126.85 | 0.977 | 145.35 | 6.310 |
| 271.85 | 1380 |  |  | 128.35 | 0.977 | 146.85 | 7.586 |
| 272.85 | 1585 |  |  | 129.35 | 1.230 | 147.35 | 7.413 |
| 272.85 | 1514 |  |  | 131.35 | 1.479 | 147.85 | 8.511 |
|  |  |  |  | 133.35 | 1.698 | 148.85 | 9.550 |
| eq. 1a | $\mathrm{P} / \mathrm{kPa}$ |  |  | 134.35 | 1.950 | 150.35 | 9.120 |

TABLE 2.1.1.1.37.1 (Continued)
Piacente et al. 1991

| transpiration method |  | torsion method |  | torsion (continued) |  | torsion (continued) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $t /{ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| A | $18.63 \pm 1.03$ |  |  | 135.35 | 2.188 | 150.85 | 10.00 |
| B | $9892 \pm 552$ |  |  | 136.35 | 2.455 | 151.85 | 10.47 |
|  |  |  |  | 137.35 | 2.951 | 152.35 | 12.88 |
|  |  |  |  | 138.35 | 3.467 | 152.85 | 13.18 |
|  |  |  |  | 139.35 | 3.890 | 153.85 | 14.13 |
|  |  |  |  | 141.35 | 4.677 | 155.85 | 15.85 |
|  |  |  |  | 143.35 | 5.379 |  |  |
|  |  |  |  |  |  | eq. 1a | $\mathrm{P} / \mathrm{kPa}$ |
|  |  |  |  |  |  | A | $28.91 \pm 0.40$ |
|  |  |  |  |  |  | B | $14285 \pm 345$ |

3. 

Piacente et al. 1991 (cont'd)
Piacente et al. 1994

| Knudsen effusion |  | torsion-effusion |  | torsion-effusion (continued) |  | torsion-effusion (continued) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  | run a |  | run b |  | run c |  |
| 83 | 0.01995 | 146.85 | 4.01 | 117.85 | 0.320 | 118.85 | 0.320 |
| 92 | 0.04677 | 147.85 | 4.49 | 120.85 | 0.401 | 124.85 | 0.481 |
| 102 | 0.1514 | 148.85 | 5.13 | 124.85 | 0.481 | 127.85 | 0.641 |
| 111 | 0.2818 | 149.85 | 5.77 | 128.85 | 0.801 | 130.85 | 0.801 |
| 119 | 0.5623 | 150.85 | 6.42 | 131.85 | 1.120 | 133.85 | 1.12 |
|  |  | 151.85 | 7.05 | 134.85 | 1.52 | 136.85 | 1.60 |
| bp/K | 658.2 | 152.85 | 7.69 | 137.85 | 2.08 | 139.85 | 2.08 |
| $\mathrm{mp} / \mathrm{K}$ | 329.4 | 153.85 | 8.33 | 141.85 | 2.88 | 142.85 | 2.72 |
|  |  | 154.85 | 9.13 | 145.85 | 4.17 | 146.85 | 3.85 |
| eq. for transpiration, torsion |  | 155.85 | 9.61 | 149.85 | 5.77 | 151.85 | 6.09 |
| and Knudsen effusion |  | 156.85 | 10.9 | 156.85 | 10.7 | 154.85 | 7.85 |
| eq. 3a | $\mathrm{P} / \mathrm{kPa}$ | 157.85 | 11.7 | 159.85 | 13.5 | 157.85 | 10.4 |
| A | $17.76 \pm 0.46$ | 159.85 | 13.3 |  |  |  |  |
| B | $8050 \pm 460$ | 161.85 | 15.5 |  |  |  |  |
| C | $72 \pm 10$ | 163.85 | 18.9 |  |  |  |  |
|  |  |  |  | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ |
|  |  | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ | A | $13.75 \pm 0.29$ | A | $13.65 \pm 0.29$ |
|  |  | A | $14.50 \pm 0.36$ | B | $6765 \pm 119$ | B | $6748 \pm 120$ |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=60.70$ |  | B <br> temp ra | $\begin{aligned} & 7084 \pm 153 \\ & 420-437 \mathrm{~K} \end{aligned}$ | temp range: 391-433 K |  | temp range: $392-431 \mathrm{~K}$ |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\text {sub }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=177.2 \\ & \text { at } 298.15 \mathrm{~K} \end{aligned}$ |  |  | overall vapor pressure eq. |  |  |  |  |
|  |  |  |  | eq. 1 | $\mathrm{P} / \mathrm{kPa}$ |  |  |
|  |  |  |  | A | $14.01 \pm 0.30$ |  |  |
|  |  |  |  | B | $6882 \pm 50$ |  |  |
|  |  |  |  | $\begin{array}{cc} \Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)= & \\ \text { at } 414 \mathrm{~K} & 132 \pm 1 \end{array}$ |  |  |  |
|  |  |  |  | $\mathrm{mp} / \mathrm{K}$ | 329 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\text {fus }} /(\mathrm{kJ} \mathrm{m}$ | $=59.9$ |  |  |
|  |  |  |  | $\begin{aligned} & \Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ} \\ & \text { at } 298.15 \end{aligned}$ | $=191.5 \pm 1$ |  |  |



FIGURE 2.1.1.1.37.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-hexacosane.

### 2.1.1.2 Cycloalkanes

### 2.1.1.2.1 Cyclopentane



Common Name: Cyclopentane
Synonym: pentamethylene
Chemical Name: cyclopentane
CAS Registry No: 287-92-37
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{10}$
Molecular Weight: 70.133
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -93.4 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
49.3 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.7457 (Weast 1984)
$0.7454,0.7440 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$94.10 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density; McAuliffe 1966)
99.5 (calculated-Le Bas method at normal boiling point, Abernethy et al. 1988; Mackay \& Shiu 1990)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
28.527, $27.296\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$0.609 \quad$ (Riddick et al. 1986)
$4.9,0.34,0.60 ; 5.84\left(-151.15,-135.15,-93.45^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
45.96, 40.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
156 (shake flask-GC, McAuliffe 1963, 1966)
342* (shake flask-GC, measured range $5.11-45.21^{\circ} \mathrm{C}$, Pierotti \& Liabastre 1972)
160* (shake flask-GC, measured range $25-153.1^{\circ} \mathrm{C}$, Price 1976)
160 (shake flask-GC, Krzyzanowska \& Szeliga 1978)
164 (shake flask-GC, Groves 1988)
156* (IUPAC "tentative" best, IUPAC Solubility Data Series, Shaw 1989)
166* (calculated-liquid-liquid equilibrium LLE data, temp range 273.2-426.3 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
27250* $\quad\left(14.25^{\circ} \mathrm{C}\right.$, static method-manometry, measured range -47.24 to $14.25^{\circ} \mathrm{C}$, Ashton et al. 1943)
$34890^{*} \quad\left(20.2^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $15.7-50^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87798-1119.208 /\left(230.738+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.7-50.0^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
43150* (Antoine eq. regression, temp range -68 to $49.4^{\circ} \mathrm{C}$, Stull 1947)
42330 (calculated from exptl. determined data, Dreisbach 1955; quoted, Hine \& Mookerjee 1975)
$\log (\mathrm{P} / \mathrm{mmHg})=6,88676-1124.162 /\left(231.361+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -25 to $110^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
29036* (selected exptl. data, temp range -39 to $230^{\circ} \mathrm{C}$, Pasek \& Thodos 1962)

42400 (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971; quoted, Mackay \& Shiu 1981)
42330* (derived from compiled data, temp range -40.4 to $71.6^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88676-1124.162 /\left(231.361+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -40.4 to $71.6^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7411.1 /(\mathrm{T} / \mathrm{K})]+7.940722$; temp range -68 to $49.3^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=[1-322.386 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.818603-7.52365 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+8.27395 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 190.20-503.20 K (Cox eq., Chao et al. 1983)

42570, 42320 (calculated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.25832-1240.438 /\left(242.957+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -47.25 to $14^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.82877-1133.199 /\left(232.415+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range $15.7-50.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
42320 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88676-1124.162 /\left(231.36+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -40 to $72^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 ) 42400 (selected lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.04584-1142.30 /\left(233.463+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 42340 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.0080-1122.21 /(-42.011+\mathrm{T} / \mathrm{K})$; temp range $280-311 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.08918-1174.132 /(-34.864+\mathrm{T} / \mathrm{K})$; temp range $322-384 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.41769-1415.096 /(-0.66+\mathrm{T} / \mathrm{K})$ temp range $381-455 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.77782-1749.65 /(48.533+\mathrm{T} / \mathrm{K})$; temp range $452-511 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=29.1547-2.3512 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.6965 \cdot \log (\mathrm{~T} / \mathrm{K})-1.6212 \times 10^{-10} .(\mathrm{T} / \mathrm{K})+3.125 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $179-512 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$35000^{*} \quad\left(20.14^{\circ} \mathrm{C}\right.$, differential pressure gauge, measured range -68.59 to $70.06^{\circ} \mathrm{C}$, Mokbel et al. 1995)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
18800 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
13310; 18380 (calculated-group contribution, bond contribution, Hine \& Mookerjee 1975)
18500; 19100, 18600 (recommended; calculated-P/C, Mackay \& Shiu 1981)
17550 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
19030 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
16617* (27.9${ }^{\circ} \mathrm{C}$, EPICS-GC, measured range $27.9-45^{\circ} \mathrm{C}$, Hansen et al. 1993)
$\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-3351 /(\mathrm{T} / \mathrm{K})+14.0$; temp range $27.9-45^{\circ} \mathrm{C}($ EPICS-GC, Hansen et al. 1993 $)$
$12796\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001) $\log \mathrm{K}_{\mathrm{AW}}=5.162-1302 /(\mathrm{T} / \mathrm{K})$ (summary of literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
2.05 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
3.00 (shake flask-GC, Leo et al. 1975; Hansch \& Leo 1979)
3.00 (recommended, Sangster 1989, 1993)
3.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.30 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=(4.72 \pm 0.28) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ calc $)=5.80 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=5.40 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}}=5.40 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.3 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\left.\mathrm{O}^{(3} \mathrm{P}\right)$ atoms at room temp. (Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=6.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K and $5.18 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K and $5.24 \times 10^{-12}$ $\mathrm{cm}^{3} \cdot$ molecule $^{-1} \mathrm{~s}^{-1}$ at 299 K and $4.43 \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule $^{-1} \mathrm{~s}^{-1}$ at 300 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=(3.12 \pm 0.23) \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (flash photolysis-resonance absorption technique, Jolly et al. 1985)
$\mathrm{k}_{\mathrm{OH}}=5.02 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K , measured range 295-491 K (Droege \& Tully 1987)
$\mathrm{k}_{\mathrm{OH}}^{*}=5.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}=5.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ at 298 K with an estimated lifetime of 27 h in summer daylight (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}} *=5.02 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}} *=4.83 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $230-400 \mathrm{~K}$ (relative rate method, DeMore \& Bayes 1999)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $\mathrm{t}_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
photooxidation reaction rate constant $\mathrm{k}=5.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical in air at 298 K (Atkinson 1990; Altshuller 1991) with an estimated lifetime of 27 h , based on reaction rate with OH radical in summer daylight (Altshuller 1991).

TABLE 2.1.1.2.1.1
Reported aqueous solubilities of cyclopentane at various temperatures

| Pierotti \& Liabastre 1972 | Price 1976 | Shaw 1989a |  | Ma̧czyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC/FID | shake flask-GC/FID | IUPAC | ve" values | calc-rec | d LLE data |
| $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad \mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{\mathbf{- 3}}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{C} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 5.11338 .6 | $25.0 \quad 160$ | 5 | 339 | 25 | 168 |
| $15.21 \quad 341.7$ | 40.1 | 15 | 342 | 40.1 | 175 |
| $25.11 \quad 341.9$ | 55.7180 | 25 | 156 | 55.7 | 195 |
| $35.21 \quad 368.5$ | 99.1 296 | 30 | 160 | 99.1 | 343 |
| $45.21 \quad 341.5$ | 118.0 372 | 40 | 350 | 118 | 468 |
|  | 137.3 611 | 60 | 500 | 137.3 | 701 |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=-2.50$ | 153.1 | 80 | 750 | 153.1 | 974 |
| $25^{\circ} \mathrm{C}$ |  | 100 | 1100 |  |  |
|  | $\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=-2.80$ | 120 | $1600$ |  |  |
|  | $25^{\circ} \mathrm{C}$ | 140 | $2600$ |  |  |
|  |  | 160 | 3850 |  |  |
|  |  | 180 | 6700 |  |  |
|  |  | 200 | 14000 |  |  |



FIGURE 2.1.1.2.1.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for cyclopentane.

TABLE 2.1.1.2.1.2
Reported vapor pressures of cyclopentane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D}\left[\mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}\right]$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} / \mathrm{T}(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \times 10^{-3}(\mathrm{~T} / \mathrm{K})-\mathrm{E} \times 10^{-8}(\mathrm{~T} / \mathrm{K})^{2}$
1.

| Ashton et al. 1943 |  | Willingham et al. 1945 |  | Stull 1947 |  | Pasek \& Thodos 1962 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static method-manometry |  | ebulliometry |  | summary of literature data |  | selected experimental data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| -47.24 | 830.6 | 15.707 | 28956 | -68.0 | 133.3 | -39.064 | 1571 |
| -38.35 | 1570 | 20.196 | 34892 | -49.6 | 666.6 | 9.335 | 21949 |
| -31.63 | 2446 | 25.598 | 43322 | -40.4 | 1333 | 15.722 | 29036 |
| -24.7 | 3753 | 31.172 | 53656 | -30.1 | 2666 | 48.146 | 97608 |
| -18.6 | 5360 | 37.119 | 66760 | -18.6 | 5333 | 57.885 | 133322 |
| -12.91 | 7350 | 43.574 | 83722 | -11.3 | 7999 | 71.612 | 1999836 |
| -7.29 | 9875 | 48.131 | 97608 | -1.30 | 13332 | 100.005 | 4197790 |
| -1.93 | 12931 | 48.621 | 99205 | 13.8 | 26664 | 230.065 | 4023402 |
| 4.47 | 17569 | 49.073 | 100698 | 31.0 | 53329 |  |  |
| 9.33 | 21949 | 49.587 | 102401 | 49.3 | 101325 | bp/ ${ }^{\circ} \mathrm{C}$ | 49.307 |
| 14.25 | 27250 | 50.031 | 103921 |  |  |  |  |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 49.20 |  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -93.7 | Frost-K derived | rf equation: exptl. data |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -93.62 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 49.262 |  |  | eq 5 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 21.62180 |
| eq. 6 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | B | -2131.85 |
| A | 30.957385 | A | 6.87798 |  |  | C | -4.83947 |
| B | 2298.386 | B | 1119.208 |  |  | D | 1.41701 |
| C | 8.91170 | C | 230.738 |  |  |  |  |
| D | 4.385677 |  |  |  |  | Frost-K | rf equation: |
| E | 1.054940 |  |  |  |  | calculat structure | m molecular mal bp and |

TABLE 2.1.1.2.1.2 (Continued)

| Ashton et al. 1943 | Willingham et al. 1945 |  | Stull 1947 |  | Pasek \& Thodos 1962 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static method-manometry | ebulliometry |  | summary of literature data |  | selected experimental data |  |
| $\mathbf{t /}{ }^{\circ} \mathbf{C} \quad \mathbf{P} / \mathbf{P a}$ | $t^{\prime}{ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{2} \mathrm{C}$ | P/Pa |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=29.21 \\ & \text { at } 25^{\circ} \mathrm{C} \end{aligned}$ |  |  |  |  | deviations of resulting v.p.:- |  |
|  |  |  |  |  | eq 5 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  | A | 21.63300 |
|  |  |  |  |  | B | -2132.5 |
|  |  |  |  |  | C | -4.84313 |
|  |  |  |  |  | D | 1.41701 |

2. 

| Zwolinski \& Wilhoit 1971 |  | Mokbel et al. 1995 |  |
| :---: | :---: | :---: | :---: |
| selected values |  | static method-manometry |  |
| $t^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |
| -40.4 | 1333 | -68.59 | 138 |
| -30.1 | 2666 | -59.24 | 313 |
| -23.6 | 4000 | -49.42 | 692 |
| -18.6 | 5333 | -39.51 | 1446 |
| -14.7 | 6666 | -39.42 | 1456 |
| -11.3 | 7999 | -29.66 | 2775 |
| -5.80 | 10666 | -29.53 | 2781 |
| -1.30 | 13332 | -19.77 | 5034 |
| 7.28 | 19998 | -19.64 | 5057 |
| 13.78 | 26664 | -9.86 | 8679 |
| 19.08 | 33331 | -9.73 | 8718 |
| 23.57 | 39997 | 0.15 | 14340 |
| 31.01 | 53329 | 0.22 | 14430 |
| 37.08 | 66661 | 10.11 | 22750 |
| 42.35 | 79993 | 10.17 | 22840 |
| 46.78 | 93326 | 20.08 | 34860 |
| 47.627 | 95992 | 20.14 | 35000 |
| 48.453 | 98659 | 30.27 | 51930 |
| 49.262 | 101325 | 40.23 | 74670 |
|  |  | 50.14 | 104580 |
|  |  | 60.12 | 143100 |
| eq. 2 | P/mmHg | 65.10 | 166090 |
| A | 6.88676 | 70.06 | 191640 |
| B | 1124.162 |  |  |
| C | 231.361 | Wagner | en in ref. |
| bp/ ${ }^{\circ} \mathrm{C}$ | 49.262 |  |  |
| $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  |
| at $25^{\circ} \mathrm{C}$ | 28.53 |  |  |
|  | 27.30 |  |  |



FIGURE 2.1.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for cyclopentane.
TABLE 2.1.1.2.1.3
Reported Henry's law constants of cyclopentane at various temperatures

| Hansen et al. $\mathbf{1 9 9 3}$ |  |
| :---: | :---: |
|  | EPICS-GC |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{k P a ~ m}^{3} / \mathrm{mol}\right)$ |
| 27.9 | 16.617 |
| 35.8 | 24.318 |
| 45.0 | 30.398 |
| $\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
|  | $\mathrm{H} /(\mathrm{kPa} \mathrm{m} 3 / \mathrm{mol})$ |
| A | $14 \pm 2.03$ |
| B | $3351 \pm 633$ |



FIGURE 2.1.1.2.1.3 Logarithm of Henry's law constant versus reciprocal temperature for cyclopentane.

### 2.1.1.2.2 Methylcyclopentane



Common Name: Methylcyclopentane
Synonym:
Chemical Name: methylcyclopentane
CAS Registry No: 96-37-3
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{12}$
Molecular Weight: 84.159
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -142.42 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 71.8 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $25^{\circ} \mathrm{C}$ ):
0.7487, $0.7439 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$112.4,113.1 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated from density)
121.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 41.59, $29.08 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
6.929 (Riddick et al. 1986)
6.93 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
53.01, 43.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

| 42.6 | (shake flask-GC, McAuliffe 1963) |
| :--- | :--- |
| 42.0 | (shake flask-GC, McAuliffe 1966) |
| 41.8 | (shake flask-GC, Price 1976) |
| 45.0 | (partition coefficient-GC, Rudakov \& Lutsyk 1979) |
| 43.0 | (recommended, IUPAC Solubility Data Series, Shaw 1989) |
| 74.8 | (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004) |

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$16680 \quad\left(22.75^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $15.0-22.6^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86283-1186.059 /\left(229.042+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.0-22.6^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
17870 (Antoine eq. regression, temp range -53.7 to $71.8^{\circ} \mathrm{C}$, Stull 1947)
18330 (calculated from exptl. determined data, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86283-1186.059 /\left(226.042+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -5 to $125^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
18302 (interpolated-Antoine eq., temp range -23.7 to $95.7^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86283-1186.059 /\left(226.042+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -23.7 to $95.7^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
17850 (interpolated-Antoine eq., temp range -53.7 to $71.8^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7490.0 /(\mathrm{T} / \mathrm{K})]+7.945471$; temp range -53.7 to $71.8^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{atm})=[1-344.830 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.872156-9.88091 \times 10^{-4} .(\mathrm{T} / \mathrm{K})+10.8367 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 183.15-513.15 K (Cox eq., Chao et al. 1983)

18330 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.99178-1188.32 /\left(226.307+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.035-72.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
18330 (interpolated-Antoine eq., Dean 1985)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86283-1186.059 /\left(226.04+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -24 to $96^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
18400 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.98773-1186.059 /\left(226.042+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
18340 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.98551-1184.874 /(-47.232+\mathrm{T} / \mathrm{K})$; temp range $288-346 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
18400, 17066 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=32.4766-2.6434 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.733 \cdot \log (\mathrm{~T} / \mathrm{K})+2.0749 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.2158 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$; temp range 131-533 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
36664 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$ reported as exptl., Hine \& Mookerjee 1975)
22090, 27810 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
36700; 36700, 36800 (recommended, calculated-P/C, Mackay \& Shiu 1981)
25370 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
36934 (calculated-P/C, Eastcott et al. 1988)
36180 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.35 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
3.37 (shake flask, Log P Database, Hansch \& Leo 1987)
3.37 (recommended, Sangster 1989)
3.37 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=7.10 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson 1990, 1991)
$\mathrm{k}_{\mathrm{OH}}=7.10 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a estimated lifetime $\tau=20 \mathrm{~h}$ in summer daylight (Altshuller 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $\mathrm{t}_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
rate constant $\mathrm{k}=7.10 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with hydroxyl radical in air (Atkinson 1990, 1991, Altshuller 1991); and an estimated reaction lifetime $\tau=20 \mathrm{~h}$ in summer daylight (Altshuller 1991).

### 2.1.1.2.3 1,1,3-Trimethylcyclopentane



Common Name: 1,1,3-Trimethylcyclopentane
Synonym:
Chemical Name: 1,1,3-trimethylcyclopentane
CAS Registry No: 4516-69-2
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16}$
Molecular Weight: 112.213
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-142.4 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
104.9 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7483,0.7430\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$146.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Wang et al. 1992)
166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
36.23, $32.35\left(25^{\circ} \mathrm{C}\right.$, bp, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
3.73 (shake flask-GC, Price 1976)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.80948-1275.998 /\left(219.899+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $28.9-105.8^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
5300 (calculated from determined data, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80947-1275.988 /\left(219.899+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-140^{\circ} \mathrm{C}$ (interpolated-Antoine eq. for liquid state, Dreisbach 1955)
5300 (interpolated-Antoine eq., temp range -0.30 to $131.3^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80947-1275.998 /\left(219.899+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -0.30 to $131.3^{\circ} \mathrm{C}$ (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{atm})=[1-378.056 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.848231-8.28174 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+8.81168 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$
272.85-404.45 K (interpolated-Cox eq., Chao et al. 1983)

5300 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.93423-1275.928 /\left(219.893+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $28.944-105.8^{\circ} \mathrm{C}$ (extrapolated-Antoine eq. from reported exptl. data, Boublik et al. 1984)
5070 (extrapolated-Antoine eq., temp range $29-106^{\circ} \mathrm{C}$, Dean 1985. 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.80931-1275.92 /\left(219.89+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $29-106^{\circ} \mathrm{C}$ (extrapolated-Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93036-1273.902 /(-53.454+\mathrm{T} / \mathrm{K})$; temp range $301-379 \mathrm{~K}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
159000 (calculated-P/C, Mackay \& Shiu 1981)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.28 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
3.34 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Air: atmospheric $\mathrm{t}_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976).

### 2.1.1.2.4 n-Propylcyclopentane



Common Name: n-Propylcyclopentane Synonym:
Chemical Name: n-propylcyclopentane
CAS Registry No: 2040-96-2
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16}$
Molecular Weight: 112.213
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-117.3 (Dreisbach 1955; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
130.937 (Willingham et al. 1945)

131 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7763,07723\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$144.6 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 41.197, 34.746( $25^{\circ} \mathrm{C}$, bp, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 10.04 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 64.45, 57.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

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2.04 (shake flask-GC, Price 1976)
1.77 (shake flask-GC, Krzyzanowska & Szeliga 1978)
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Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.89887-1380.391 /\left(212.610+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $51.7-131.9^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.30392-1384.386 /\left(213.159+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $51.9-131.9^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
1650 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90392-1384.386 /\left(213.159+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $40-170^{\circ} \mathrm{C}$ (extrapolated-Antoine eq. for liquid state, Dreisbach 1955)
1640 (interpolated-Antoine eq., temp range -21.3 to $158.2^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.30392-1384.386 /\left(213.159+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -21.3 to $158.2^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
1646 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91061-1388.511 /\left(213.615+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $51.88-131.97^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1973)
1640, 5320 (quoted, calculated-bp, Mackay et al. 1982)
$\log (\mathrm{P} / \mathrm{atm})=[1-427.713 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.865420-7.04026 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+5.98562 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$
313.35-458.95 K (Cox eq., Chao et al. 1983)

1644 (extrapolated-Antoine eq., temp range $40-186^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88646-1460.80 /\left(207.94+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $40-186^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.04236-1393.284 /(-58.949+\mathrm{T} / \mathrm{K})$; temp range $323-406 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=33.922-3.2097 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.9914 \cdot \log (\mathrm{~T} / \mathrm{K})-3.2992 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+2.0684 \times 10^{-6}$. $(\mathrm{T} / \mathrm{K})^{2}$; temp range $156-603 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
90200 (calculated-P/C, Mackay \& Shiu 1981)
90430 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.95 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
2.65 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
4.37 (calculated-fragment const., Müller \& Klein 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1 / 2}$ :

Half-Lives in the Environment:

### 2.1.1.2.5 Penty/cyclopentane



Common Name: Pentylcyclopentane
Synonym: 1-cyclopentylpentane
Chemical Name: pentylcyclopentane
CAS Registry No: 3741-00-2
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{20}$
Molecular Weight: 140.266
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-83 (Dreisbach 1955; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
180 (Dreisbach 1955; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.7912,0.7874 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
177.3, $178.1\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
210.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
51.12, 39.94 ( $25^{\circ}$, bp, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.115 (shake flask-GC, Price 1976)
0.13 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
159 (calculated by formula, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.929-1526.0 /\left(197.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $85-220^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

152 (extrapolated-Antoine eq., temp range $60-210^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9414-1540.6 /\left(198.8+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $60-210^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
18500 (calculated-P/C, Mackay \& Shiu 1981)
18600 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 2.1.1.2.6

 Cyclohexane

Common Name: Cyclohexane
Synonym: hexahydrobenzene, hexamethylene
Chemical Name: cyclohexane
CAS Registry No: 110-82-7
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{12}$
Molecular Weight: 84.159
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
6.59 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
80.73 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.7786,0.7739 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$108.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Lande \& Banerjee 1981)
118.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 32.89, $30.05 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
2.677 (Riddick et al. 1986)
5.84, 2.68; $9.41 \quad\left(-87.05,6.65^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
45.77, 44.55 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$, additional data at other temperatures designated $*$ are compiled at the end of this section.):
80.0 (shake flask-gravitational method, McBain \& Lissant 1951)
55.0 (shake flask-GC, McAuliffe 1963, 1966)
$88.84^{*} \quad$ (shake flask-GC/FID, measured range $5.11-45.21^{\circ} \mathrm{C}$, Pierotti \& Liabastre 1972)
56.7 (shake flask-GC/FID, Leinonen \& Mackay 1973)
57.5 (shake flask-vapor extraction-GC/FID, Mackay \& Shiu 1975)
55.8, 50.2, 61.7 (shake flask-GC, Mackay et al. 1975)
66.5 (shake flask-GC/FID, Price 1976)
66.5 (shake flask-GC, Krzyzanowski \& Szeliga 1978)
$52.0 \quad\left(23.5^{\circ} \mathrm{C}\right.$, elution chromatography, Schwarz 1980)
72.4 (calculated-HPLC- $\mathrm{k}^{\prime}$ correlation, converted from reported $\gamma_{\mathrm{w}}$, Hafkenscheid \& Tomlinson 1983)
$72.8^{*} \quad\left(40^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $40-209.06^{\circ} \mathrm{C}$, Tsonopoulos \& Wilson 1983)
58.4 (shake flask-GC, Groves 1988)
58.0* (IUPAC recommended best value, Shaw 1989a)
$\ln x=-301.366+12924.45 /(\mathrm{T} / \mathrm{K})+43.2980 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)
$\ln x=-219.863+6693.78 /(\mathrm{T} / \mathrm{K})+31.3744 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from direct fit of solubility data, Tsonopoulos 2001)
60.78 (calculated-liquid-liquid equilibrium LLE data, temp range 278.2-482.2 K, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
12972 (gas saturation/air-bubbling method, Washburn \& Handorf 1935)
$16212^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, vapor-liquid equilibrium VLE data, measured range $30-80^{\circ} \mathrm{C}$, Scatchard et al. 1939)
$\log (\mathrm{P} / \mathrm{mmHg})=6.65859-1040.641 /(\mathrm{T} / \mathrm{K})-104.865 /(\mathrm{T} / \mathrm{K})^{2}$; temp range $30-60^{\circ} \mathrm{C}(\mathrm{VLE}$ data, Scatchard et al. 1939)

10910* $\quad\left(20.97^{\circ} \mathrm{C}\right.$, manometry, measured range $6.33-20.97^{\circ} \mathrm{C}$, Aston et al. 1943 b$)$
$11700^{*} \quad\left(20.96^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $19.9-81.6^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84498-1203.526 /\left(222.863+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $19.9-81.6^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
12280* (calculated-Antoine eq. regression, temp range -45.3 to $80.7^{\circ} \mathrm{C}$, Stull 1947)
10253*; $10375\left(20.015^{\circ} \mathrm{C}\right.$, selected exptl., calculated-Frost-Kalkwarf vapor pressure eq., temp range 293.185-551.225 K, Pasek \& Thodos 1962)
$\log (\mathrm{P} / \mathrm{mmHg})=23.14002-2411.8 /(\mathrm{T} / \mathrm{K})-5.17900 \cdot \log (\mathrm{~T} / \mathrm{K})+1.84394 \cdot\left[(\mathrm{P} / \mathrm{mmHg}) /(\mathrm{T} / \mathrm{K})^{2}\right] ;$ temp range 293.185-551.225 K (Frost-Kalkwarf eq., Pasek \& Thodos 1962)

13040* (static method, measured range $25-75^{\circ} \mathrm{C}$, Cruickshank \& Cutler 1967)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85875-1212.014 /\left(233.956+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25-75^{\circ} \mathrm{C}$ (static method, Cruickshank \& Cutler 1967)
13010 (calculated from determined data, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84498-1203.526 /\left(222.863+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -20 to $142^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
13159* $\quad\left(25.26^{\circ} \mathrm{C}\right.$, temp range $17.55-80.22^{\circ} \mathrm{C}$, Boublik 1960; quoted, Boublik et al. 1984)
13014* (interpolated-Antoine eq., temp range $6.59-105.2^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84130-1201.531 /\left(222.647+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $6.59-105.2^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
11170 (interpolated-Antoine eq., temp range -45.3 to $257.5^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7830.9 /(\mathrm{T} / \mathrm{K})]+7.662126$; temp range -45.3 to $257.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{atm})=[1-353.663 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.881199-9.58655 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+9.72305 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; temp range 227.85-553.64 K (Cox eq., Chao et al. 1983)

13010, 13040 (interpolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.97561-1206.731 /\left(223.223+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range $19.9-81.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.98226-1211.248 /\left(223.869+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25-75^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.00569-1223.273 /\left(225.089+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $17.55-80.22^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Cruickshank \& Cutler 1967, Boublik et al. 1984)
13020 (interpolated-Antoine eq., temp range $20-81^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84130-1201.53 /\left(222.65+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-81^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
13040 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.96407-1200.31 /\left(222.504+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
13070 (interpolated-Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=7.2778-1747.2 /(26.84+\mathrm{T} / \mathrm{K})$; temp range $223-280 \mathrm{~K}$ (Antoine eq.-I, solid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.9682-1201.531 /(-50.503+\mathrm{T} / \mathrm{K})$; temp range $293-335 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.03245-1244.124 /(-44.911+\mathrm{T} / \mathrm{K})$; temp range $353-414 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.36849-1519.732 /(-4.032+\mathrm{T} / \mathrm{K})$; temp range $412-491 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.37347-2683.075 /(159.31+\mathrm{T} / \mathrm{K})$; temp range $489-533 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
12920, 1730 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=48.5529-3.0874 \times 10^{3} /(\mathrm{T} / \mathrm{K})-15.521 \cdot \log (\mathrm{~T} / \mathrm{K})+7.383 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+6.3563 \times 10^{-12} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $280-554 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$12068^{*} \quad\left(23.363^{\circ} \mathrm{C}\right.$, comparative ebulliometry, measured range $281-552 \mathrm{~K}$, data fitted to Wagner eq., Ewing \& Ochoa 2000)
16230, $36180 \quad\left(30,50^{\circ} \mathrm{C}\right.$, VLE equilibrium data, Carmona et al. 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
19860 (calculated-P/C, Mackay \& Shiu 1975)
19690 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
18380, 27810 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
18000 (recommended; Mackay \& Shiu 1981)
22092 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
5532, 17935, 19353, 1450 (bubble column non-equilibrium measurement, EPICS-GC, direct concentration. ratio, calculated-UNIFAC activity coeff., Ashworth et al. 1988)
17935* (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=9.141-3238 /(\mathrm{T} / \mathrm{K})$; temp range: $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
19980 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
$37190^{*} \quad\left(40^{\circ} \mathrm{C}\right.$, equilibrium headspace-GC, measured range $40-80^{\circ} \mathrm{C}$, Kolb et al. 1992)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=-12.90+3228 /(\mathrm{T} / \mathrm{K})$; temp range: $40-80^{\circ} \mathrm{C}$ (equilibrium headspace-GC measurements, Kolb et al. 1992)
$15062\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001) $\log \mathrm{K}_{\mathrm{AW}}=5.154-1279 /(\mathrm{T} / \mathrm{K})$ (summary of literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {Ow }}$ :
2.46
3.44
3.40
3.18, 3.48, 3.48
3.69
3.70
3.44
3.73 (from activity coefficient measurement, Tse \& Sandler 1994)
3.44 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated* are compiled at the end of this section:
2.83* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range 20.29-50.28 ${ }^{\circ} \mathrm{C}$, Gruber et al. 1997)
2.71 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
2.38 (estimated, Howard 1990)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
2.68 (estimated-S, Howard 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $\mathrm{t}_{1 / 2}=2.8 \mathrm{~h}$ from a model river 1 m deep with a $1 \mathrm{~m} / \mathrm{s}$ current and a $3 \mathrm{~m} / \mathrm{s}$ wind (Lyman et al. 1982, quoted, Howard 1990).
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}} *(\operatorname{exptl})=5.38 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=4.79 \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 295 K , measured range 295-497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=6.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K} ; \mathrm{k}_{\mathrm{OH}}($ calc $)=6.7 \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule $^{-1} \mathrm{~s}^{-1}$ at 300 K (Darnall et al. 1978)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.40 \times 10^{-13} \mathrm{~cm}^{3} \cdot$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atoms at room temp. (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=7.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{OH}}=(7.57 \pm 0.05) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984 c )
$\mathrm{k}_{\mathrm{OH}}=(6.20 \pm 0.44) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(24.4 \pm 0.4)^{\circ} \mathrm{C}$ with an atmospheric lifetime of 1.9 d for an average OH radical concentration of $1.0 \times 10^{6}$ molecules $/ \mathrm{cm}^{3}$ (Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}=7.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson 1986; quoted, Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}=7.14 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 292 K , measured range 292-491 K (Droege \& Tully 1987)
$\mathrm{k}_{\mathrm{OH}}=7.38 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Dilling et al. 1988)
$\mathrm{k}_{\mathrm{OH}} *=7.49 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=7.49 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=13.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3}=1.35 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1991)
$\mathrm{k}_{\mathrm{NO} 3}($ exptl $)=1.35 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}($ calc $)=2.04 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Aschmann \& Atkinson 1995)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=7.21 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=6.69 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $230-400 \mathrm{~K}$ (relative rate method, DeMore \& Bayes 1999)
Hydrolysis:
Biodegradation: highly resistant to biodegradation (Howard 1990);
$\mathrm{t}_{1 / 2}$ (aq. aerobic) $=672$ to 4032 h , based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991);
$\mathrm{t}_{1 / 2}($ aq. anaerobic $)=2688$ to 16280 h , based on estimated unacclimated aqueous aerobic biodegradation halflife (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);
atmospheric lifetime $\tau=1.9 \mathrm{~d}$ for an average OH radical concentration of $1.0 \times 10^{6}$ molecules $/ \mathrm{cm}^{3}$ (Edney et al. 1986);
$t_{1 / 2}=52 \mathrm{~h}$, based on photooxidation rate constant (Howard 1990);
an atmospheric lifetime $\tau \sim 19 \mathrm{~h}$ in summer daylight, based on the photooxidation reaction rate constant of $7.49 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with OH radical in air during summer daylight (Altshuller 1991);
will degrade photochemically by hydroxyl radicals with $t_{1 / 2}=52 \mathrm{~h}$ and much faster under photochemical smog conditions with $\mathrm{t}_{1 / 2}=6 \mathrm{~h}$ (Howard 1990);
$\mathrm{t}_{1 / 2}=8.7-87 \mathrm{~h}$, based on reaction with OH radical half-life in air (Howard et al. 1991).
Surface water: volatilization $\mathrm{t}_{1 / 2}=2 \mathrm{~h}$ in a model river (Howard 1990);
$t_{1 / 2}=672-4320 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
photooxidation $\mathrm{t}_{1 / 2}=1.4 \times 10^{9}$ to $6.9 \times 10^{10} \mathrm{~h}(16000$ to 780000 yr$)$, based on measured rate data for alkylperoxyl radicals in aqueous solution (Howard et al. 1991).
Ground water: $t_{1 / 2}=1344-8640 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{1 / 2}=672-4320 \mathrm{~h}$, based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991).
Biota:

TABLE 2.1.1.2.6.1
Reported aqueous solubilities of cyclohexane at various temperatures

| Pierotti \& Liabastre 1972 |  | Tsonopoulos \& Wilson 1983 |  | Shaw 1989a |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-GC |  | IUPAC recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 5.11 | 81.93 | 40 | 72.8 | 5 | - |
| 15.21 | 88.70 | 100 | 1770 | 15 | - |
| 25.11 | 88.84 | 146.89 | 4810 | 20 | - |
| 35.21 | 88.84 | 150 | 6070 | 25 | 58.0 |
| 45.21 | 91.32 | 200 | 18300 | 45 | - |
|  |  | 209.06 | 23000 | 50 | - |
|  |  |  |  | 56 | - |
|  |  |  |  | 70 | - |
|  |  |  |  | 71 | - |



FIGURE 2.1.1.2.6.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for cyclohexane.

TABLE 2.1.1.2.6.2
Reported vapor pressures of cyclohexane at various temperatures and the coefficients for the vapor pressure equations:

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| :--- | ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(1)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ |  |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (3) | (4) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D}\left[\mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}\right]$ |  |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} / \mathrm{T}(\mathrm{T} / \mathrm{K})-\mathrm{C} /(\mathrm{T} / \mathrm{K})^{2}$ |  | (5) |  |
|  |  | (6) |  |

1. 


2.

| Boublik 1960 |  | Cruickshank \& Cutler 1966 |  | Zwolinski \& Wilhoit 1971 |  | Ewing \& Ochoa 2000 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| in Boublik et al. 1984 |  | static method-manometry |  | selected values |  | comparative ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 17.55 | 9210 | 25 | 13040 | 6.69 | 5333 | 8.188 | 5777 |
| 20.16 | 10426 | 35 | 20104 | 11.01 | 6666 | 9.698 | 6243 |
| 22.98 | 11876 | 45 | 30008 | 14.66 | 7999 | 11.356 | 6791 |
| 25.26 | 13159 | 55 | 43538 | 20.666 | 10666 | 15.215 | 8225 |
| 28.77 | 15372 | 65 | 61551 | 25.536 | 13332 | 17.163 | 9039 |
| 32.77 | 18252 | 75 | 85012 | 34.904 | 19998 | 19.868 | 10284 |
| 37.10 | 21891 |  |  | 41.991 | 26664 | 22.608 | 11675 |
| 40.66 | 25264 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 6.55 | 47.763 | 33331 | 23.263 | 12086 |
| 45.77 | 30864 | bp/ ${ }^{\circ} \mathrm{C}$ | 80.728 | 52.669 | 39997 | 28.346 | 15109 |
| 50.96 | 37543 | density, $\mathrm{d}^{25}$ | 0.77386 | 60.784 | 53329 | 44.379 | 29290 |
| 56.18 | 45356 |  |  | 67.415 | 66661 | 49.393 | 35456 |
| 62.46 | 56448 | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  | 73.067 | 79993 | 55.302 | 44015 |
| 68.71 | 69467 | at $20^{\circ} \mathrm{C}$ | 33.23 | 78.021 | 93326 | 60.881 | 53541 |
| 75.42 | 86053 | $25^{\circ} \mathrm{C}$ | 32.97 | 78.944 | 95992 | 66.269 | 64227 |
| 80.22 | 99818 | $54.1{ }^{\circ} \mathrm{C}$ | 31.45 | 79.848 | 98659 | 71.034 | 75023 |
|  |  | $73.3{ }^{\circ} \mathrm{C}$ | 30.44 | 80.292 | 99992 | 75.094 | 86306 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 80.731 | $80.7^{\circ} \mathrm{C}$ | 30.03 | 80.732 | 101325 | 78.498 | 94753 |
|  |  |  |  |  |  | 80.80 | 101589 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 83.489 | 110504 |
|  |  | A | 6.85875 | A | 6.84130 | 87.149 | 122451 |
|  |  | B | 1212.014 | B | 1201.531 |  |  |
|  |  | C | 233.956 | C | 222.647 |  |  |
|  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 80.732 | temp range 281-552 K data fitted to Wagner eq. |  |
|  |  |  |  | $\begin{gathered} \Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)= \\ \text { at } 25^{\circ} \mathrm{C} \\ \text { at bp } \end{gathered}$ | $\begin{aligned} & 33.04 \\ & 29.96 \end{aligned}$ |  |  |



FIGURE 2.1.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexane.

TABLE 2.1.1.2.6.3
Reported Henry's law constants and octanol-air partition coefficients of cyclohexane at various temperatures and temperature dependence equations

$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

Henry's law constant

| Ashworth et al. 1988 |  | Kolb et al. 1992 |  | Gruber et al. 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| EPICS-GC |  | equilibrium headspace-GC |  | GC det'd activity coefficient |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} \mathrm{K}_{\text {OA }}$ |
| 10 | 10436 | 40 | 37190 | 20.29 | 2.835 |
| 15 | 12767 | 60 | 55400 | 30.3 | 2.652 |
| 20 | 14189 | 70 | 95100 | 40.4 | 2.511 |
| 25 | 17935 | 80 | 146800 | 50.28 | 2.365 |
| 30 | 22595 |  |  |  |  |
|  |  | eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ |  |  |
|  |  | A | -12.90 |  |  |
| eq. 4 a | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m} /{ }^{3} \mathrm{~mol}\right)$ | B | -3228 |  |  |
| A | 9.141 |  |  |  |  |
| B | 3238 |  |  |  |  |



FIGURE 2.1.1.2.6.3 Logarithm of Henry's law constant versus reciprocal temperature for cyclohexane.


FIGURE 2.1.1.2.6.4 Logarithm of $\mathrm{K}_{\mathrm{OA}}$ versus reciprocal temperature for cyclohexane.

### 2.1.1.2.7 Methylcyclohexane



Common Name: Methylcyclohexane
Synonym: hexahydrotoluene, cyclohexylmethane
Chemical Name: methylcyclohexane
CAS Registry No: 108-87-2
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{14}$
Molecular Weight: 98.186
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -126.6 (Dreisbach 1959; Weast 1984; Riddick et al. 1986; Stephenson \& Malanowski 1987; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 100.93 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7694,0.7651\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$127.6\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 35.359, $31.13\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 6.757 (Riddick et al. 1986) 6.75 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 46.1, 47.3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
14.0 (shake flask-GC, McAuliffe 1963, 1966)
16.0* (shake flask-GC, measured range $25-149.5^{\circ} \mathrm{C}$, Price 1976; quoted, Eastcott et al. 1988)
15.3 (partition coefficient-GC, Rudakov \& Lutsyk 1979)
15.2 $\quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, Burris \& MacIntyre 1986)
16.7 (shake flask-GC, Groves 1988)
15.1* (IUPAC recommended, temp range $25-150^{\circ}$ C, Shaw 1989)
15.82* (calculated-liquid-liquid equilibrium LLE data, temp range 298.2-410.5 K, Ma̧czyński et al. 2004)
$16.15^{*} \quad\left(26.1^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $26.1-170.8^{\circ} \mathrm{C}$, Marche et al. 2004)
$\ln (\mathrm{S} / \mathrm{ppm})=13.091-7085.522 /(\mathrm{T} / \mathrm{K})+1055594 /(\mathrm{T} / \mathrm{K})^{2}($ Marche et al. 2004 $)$
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
6128 (interpolated-Antoine eq., Stuckey \& Saylor 1940)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95423-1336.93 /(\mathrm{T} / \mathrm{K}-45.52)$; temp range $4-75^{\circ} \mathrm{C}$ (Antoine eq. based on exptl. data,
Ramsay-Young method-Hg manometer, Stuckey \& Saylor 1940)
6354* $\quad\left(25.59^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82689-1272.864 /\left(221.630+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25.6-101.8^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
5887* (calculated-Antoine eq. regression, temp range -35.9 to $100.0^{\circ} \mathrm{C}$, Stull 1947)
6180 (calculated from determined data, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82689-1272.864 /\left(221.630+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10-155^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
10207* (35.901 ${ }^{\circ} \mathrm{C}$, temp range $35.901-95.946^{\circ} \mathrm{C}$, Varushchenko et al. 1970)

6180* (interpolated-Antoine eq., temp range -3.20 to $127.0^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82300-1272.763 /\left(221.416+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -3.20 to $127.0^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
5880 (interpolated-Antoine eq., temp range -35.9 to $100^{\circ} \mathrm{C}$, Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8549.2 /(\mathrm{T} / \mathrm{K})]+7.909762$; temp range -35.9 to $100^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
5806 (calculated-bp, Mackay et al. 1982)
$\log (\mathrm{P} / \mathrm{atm})=[1-373.957 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.862568-8.71426 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+8.69685 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range
203.20-563.20 K (Cox eq., Chao et al. 1983)

5364, 6111, 6177 (Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.95366-1273.962 /\left(221.755+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25.6-101.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.95497-1275.047 /\left(221.678+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35.9-95.9^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.92856-1253.199 /\left(216.058+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $58.645-113.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Meyer et al. 1976, Boublik et al. 1984)
6180 (interpolated-Antoine eq., temp range -3 to $127^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82300-1270.763 /\left(221.42+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -3 to $127^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 ) $6100 \quad$ (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.94790-1270.763 /\left(221.416+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 6160 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.9428-1266.954 /(-52.282+\mathrm{T} / \mathrm{K})$; temp range $308-368 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.14677-1413.495 /(-32.726+\mathrm{T} / \mathrm{K})$; temp range $373-511 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.29186-2700.205 /(147.549+\mathrm{T} / \mathrm{K})$; temp range $501-573 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=38.0955-3.0738 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.684 \cdot \log (\mathrm{~T} / \mathrm{K})-5.1766 \times 10^{-11} .(\mathrm{T} / \mathrm{K})+3.5282 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $147-572 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
5205* $\quad\left(21.46^{\circ} \mathrm{C}\right.$, static method-manometry, measured range -76.96 to $41.44^{\circ} \mathrm{C}$, Mokbel et al. 1995)
$\ln x=-328.666+14073.29 /(\mathrm{T} / \mathrm{K})+47.1467 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)
$\ln x=-491.070+22132.10 /(\mathrm{T} / \mathrm{K})+70.9150 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from direct fit of solubility data, Tsonopoulos 2001)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
44080 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
31030, 41340 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
40000 (recommended; Mackay \& Shiu 1981)
31934 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
37930 (calculated-P/C, Eastcott et al. 1988)
43300 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
12666* $\quad\left(27.3^{\circ} \mathrm{C}\right.$, EPICS-GC, measured range $27.3-45^{\circ} \mathrm{C}$, Hansen et al. 1993)
$\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-9406 /(\mathrm{T} / \mathrm{K})+34.0$; temp range $27.3-45^{\circ} \mathrm{C}$ (EPICS-GC, Hansen et al. 1993)
$6410 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=13.507-3836 /(\mathrm{T} / \mathrm{K})$ (summary of literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
2.76 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
2.96 (calculated- MCI $\pi$, Murray et al. 1975)
2.82 (Hansch \& Leo 1979)
3.88 (recommended, Sangster 1989. 1993)
4.10 (calculated-fragment const. per Lyman 1982, Thoms \& Lion 1992)
2.89 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.87 (calculated-fragment const., Müller \& Klein 1992)
3.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
$3.14^{*} \quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range 20.29-50.28 ${ }^{\circ} \mathrm{C}$ Gruber et al. 1997)
3.05 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(10.6 \pm 0.3) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)
$\mathrm{k}_{\mathrm{OH}}=1.04 \times 10^{-11} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}=1.04 \times 10^{-11} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K with an estimated half-life of 13 h (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=1.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biotransformation:
Biodegradation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: an atmospheric lifetime was estimated to be 13 h in summer daylight, based on the photooxidation rate constant of $1.04 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radicals in air (Altshuller 1991).

TABLE 2.1.1.2.7.1
Reported aqueous solubilities of methylcyclohexane at various temperatures

| Price 1976 |  | Shaw 1989a |  | Marche et al. 2004 |  | Mączyński et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Shake flask-GC |  | IUPAC recommended |  | Shake flask-GC |  | Calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  |  | 25 | 15.1 | 26.1 | 16.15 | 25 | 15.82 |
| 25.0 | 16.0 | 30 | 17.0 | 70.5 | 27.49 | 40.1 | 16.91 |
| 40.1 | 18.0 | 40 | 18.0 | 100.5 | 54.88 | 55.7 | 19.64 |
| 55.7 | 18.9 | 50 | 19.0 | 131.0 | 133.1 | 99.1 | 44.18 |
| 99.1 | 33.8 | 70 | 22.0 | 151.4 | 230.7 | 120 | 76.37 |
| 120.0 | 79.5 | 90 | 29.0 | 170.8 | 386.2 | 137.3 | 125.5 |
| 137.3 | 139 | 110 | 52.0 |  |  |  |  |
| 149.5 | 244 | 130 | 110 | $\mathrm{S}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})+\mathrm{C} /(\mathrm{T} / \mathrm{K})^{2}$ |  |  |  |
|  |  | 150 | 250 | S | $\mathrm{g} / \mathrm{m}^{3}$ |  |  |
|  |  |  |  | A | 13.091 |  |  |
|  |  |  |  | B | 7085.522 |  |  |
|  |  |  |  | C | 1055594 |  |  |



FIGURE 2.1.1.2.7.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for methylcyclohexane.

TABLE 2.1.1.2.7.2
Reported vapor pressures of methylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | ---: | :--- | ---: |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D}\left[\mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}\right]$ | $(5)$ |  |

1. 

| Willingham et al. 1945 |  | Stull 1947 |  | Varushchenko et al. 1970 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | summary of literature data |  |  |  | sele | values |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 25.585 | 6354 | -35.9 | 133.3 | 35.901 | 10207 | -3.20 | 1333 |
| 29.533 | 7655 | -14.0 | 666.6 | 45.809 | 15552 | 8.70 | 2666 |
| 32.976 | 8962 | -3.2 | 1333 | 50.799 | 19018 | 16.3 | 4000 |
| 36.089 | 10303 | 8.7 | 2666 | 55.419 | 22754 | 21.98 | 5333 |
| 38.998 | 11696 | 22.0 | 5333 | 61.644 | 28719 | 26.585 | 6666 |
| 42.929 | 13820 | 35.0 | 7999 | 67.476 | 35390 | 30.477 | 7999 |
| 47.407 | 16919 | 42.1 | 13332 | 74.177 | 44530 | 36.874 | 10666 |
| 51.964 | 19918 | 59.6 | 26664 | 81.020 | 55721 | 42.063 | 13332 |
| 56.194 | 23453 | 79.6 | 53329 | 88.101 | 69542 | 52.048 | 19998 |
| 61.857 | 28958 | 100.0 | 101325 | 93.567 | 81944 | 59.604 | 26664 |
| 67.067 | 34896 |  |  | 94.159 | 93376 | 65.758 | 33331 |
| 73.349 | 43323 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -126.4 | 94.766 | 84890 | 70.990 | 39997 |
| 79.842 | 53657 |  |  | 95.307 | 86243 | 79.646 | 53329 |
| 86.771 | 66760 |  |  | 95.946 | 87847 | 86.720 | 66661 |
| 94.299 | 83721 |  |  |  |  | 92.752 | 79993 |
| 99.614 | 97628 |  |  |  |  | 98.039 | 93326 |
| 100.185 | 99205 |  |  |  |  | 99.025 | 95992 |
| 100.715 | 100697 |  |  |  |  | 99.989 | 98659 |
| 101.312 | 102398 |  |  |  |  | 100.464 | 99992 |
| 101.832 | 103919 |  |  |  |  | 100.934 | 101325 |


| TABLE 2.1.1.2.7.2 (Continued) |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Willingham et al. 1945 |  | Stull 1947 |  | Varushchenko et al. 1970 |  | Zwolinski \& Wilhoit 1971 |  |
| ebulliometry |  | summary of literature data |  |  |  | selected values |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t^{\prime}{ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 100.715 | 100697 |  |  |  |  | 99.989 | 98659 |
| 101.312 | 102398 |  |  |  |  | 100.464 | 99992 |
| 101.832 | 103919 |  |  |  |  | 100.934 | 101325 |
| bp/ ${ }^{\circ} \mathrm{C}$ | 100.934 |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 6.82300 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  | B | 1270.763 |
| A | 6.82689 |  |  |  |  | C | 221.416 |
| B | 1272.864 |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 100.934 |
| C | 221.630 |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 35.36 |
|  |  |  |  |  |  | at bp | 31.13 |

2. 

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| static method-manometry |  |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| -76.96 | 1.68 | -28.28 | 240 | 21.46 | 5205 |
| -67.0 | 5.87 | -18.38 | 497 | 31.45 | 8368 |
| -58.55 | 15.8 | -8.44 | 970 | 41.44 | 12950 |
| -48.64 | 42.4 | 1.50 | 1785 |  |  |
| -38.15 | 108 | 11.47 | 3128 | data fitted to Wagner eq. |  |



FIGURE 2.1.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for methylcyclohexane.

TABLE 2.1.1.2.7.3
Reported Henry's law constants and octanol-air partition coefficients of methylcyclohexane at various temperatures and temperature dependence equations

| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (2) | $\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| $\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\ln [\mathrm{H} /(\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol})]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (4) | $\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |

$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

| Henry's law constant |  | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {OA }}$ |  |
| :---: | :---: | :---: | :---: |
| Hansen et al. 1993 |  | Gruber et al. 1997 |  |
| EPICS-GC |  | GC det'd activity coefficient |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(kPa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | . $\log \mathrm{K}_{\mathrm{OA}}$ |
| 27.3 | 12.666 | 20.29 | 3.142 |
| 35.8 | 34.653 | 30.3 | 2.943 |
| 45.0 | 72.447 | 40.4 | 2.784 |
|  |  | 50.28 | 2.632 |
| eq. 4 | $\mathrm{H} /\left(\mathrm{kPa} \mathrm{m}^{3} / \mathrm{mol}\right)$ |  |  |
| A | $34 \pm 3.39$ |  |  |
| B | $9406 \pm 1046$ |  |  |



FIGURE 2.1.1.2.7.3 Logarithm of Henry's law constant versus reciprocal temperature for methylcyclohexane.


FIGURE 2.1.1.2.7.4 Logarithm of $K_{O A}$ versus reciprocal temperature for methylcyclohexane.

### 2.1.1.2.8 1,2,-cis-Dimethylcyclohexane



Common Name: 1,2-cis-Dimethylcyclohexane
Synonym: cis-1,2-dimethylcyclohexane
Chemical Name: 1,2-cis-dimethylcyclohexane
CAS Registry No: 2207-01-4
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16}$
Molecular Weight: 112.213
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-49.8 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
$129.8 \quad$ (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.7963, $0.7922 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$140.9 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966)
$141.6\left(25^{\circ} \mathrm{C}\right.$, calculated-density; Ruelle \& Kesselring 1997)
162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
39.715, $34.196\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
1.644 (Dreisbach 1955; Riddick et al. 1986)
8.26, 1.64 ( $-100.65,-39.05^{\circ} \mathrm{C}$, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
55.22, 50.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
6.0 (shake flask-GC, McAuliffe 1966)
5.01 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)
5.94* (generator column-GC, measured range 273.15-313.15 K, Dohányosová et al. 2004)
$\ln x=-59.7348+45.8700 / \tau+46.6282 \cdot \ln \tau ; \tau=\mathrm{T} / 298.15 \mathrm{~K}$ (empirical eq., generator column-GC, Dohányosová et al. 2004)
$\ln (\mathrm{S} / \mathrm{ppm})=11.610-8455.943 /(\mathrm{T} / \mathrm{K})+961943.2 /(\mathrm{T} / \mathrm{K})^{2}$, temp range $30.3-170^{\circ} \mathrm{C}$ (Marche et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$6352^{*} \quad\left(49.185^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $49.185-130.684^{\circ} \mathrm{C}$, Willingham et al. 1945)
$1333^{*} \quad\left(18.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -15.9 to $129.7^{\circ} \mathrm{C}$, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84164-1369.525 /\left(216.040+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $49.2-130.7^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
1929 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84164-1369.525 /\left(216.040+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $40-170^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1933* (interpolated-Antoine eq., temp range $18.4-157.6^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83746-1367.311 /\left(215.835+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $18.4-157.6^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9364.9 /(\mathrm{T} / \mathrm{K})]+8.001159$; temp range -15.9 to $129.7^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} /$ atm $)=[1-402.894 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.841813-8.56119 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+5.01855 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 257.25-430.75 K (Cox eq., Chao et al. 1983)

1927 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.96885-1370.962 /\left(216.202+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $49.2-130.68^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
1928 (interpolated-Antoine eq., temp range $18-158^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83746-1367.311 /\left(215.84+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $18-158^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{kPa})=5.96654-1369.525 /\left(216.040+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.96232-1367.306 /(-57.314+\mathrm{T} / \mathrm{K})$; temp range $322-405 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=32.1535-3.0728 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.4344 \cdot \log (\mathrm{~T} / \mathrm{K})+6.8943 \times 10^{-10} .(\mathrm{T} / \mathrm{K})+1.9558 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $223-606 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$36000 \quad$ (calculated-P/C, Mackay \& Shiu 1981)
$35830 \quad$ (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
53000, 62270 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
$44080 \quad$ (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
36045 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
36180* (derived from solute fugacity and mole fraction solubility, temp range 273.15-313.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.06 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
3.33 (calculated-MCI $\chi$, Murray et al. 1975)
3.21 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :

Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.8.1
Reported aqueous solubilities and Henry's law constants of 1,2-cis-dimethylcyclohexane at various temperatures

| Aqueous solubility |  |  |  | Henry's law constant |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Dohányosová et al. 2004 |  |  |  | Dohányosová et al. 2004 |  |
| generator column-GC/FID |  | smoothed raw exptl data |  | from solute fugacity $f$ and $x$ |  |
| T/K | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
|  | raw data |  |  |  |  |
| 274.15 | 6.608 | 273.15 | 6.59 | 273.15 | 7218 |
| 274.15 | 6.670 | 278.15 | 6.27 | 278.15 | 10566 |
| 274.15 | 6.421 | 283.15 | 6.05 | 283.15 | 14994 |
| 278.15 | 6.184 | 288.15 | 5.93 | 288.15 | 20700 |
| 278.15 | 6.234 | 293.15 | 5.90 | 293.15 | 27720 |
| 278.15 | 6.078 | 298.15 | 5.94 | 298.15 | 36180 |
| 283.75 | 6.159 | 303.15 | 6.06 | 303.15 | 46260 |
| 283.75 | 6.041 | 308.15 | 6.25 | 308.15 | 57780 |
| 288.15 | 5.767 | 313.15 | 6.51 | 313.15 | 70740 |
| 288.15 | 6.234 |  |  |  |  |
| 288.15 | 6.147 | $\ln x=$ | $+\mathrm{C} \ln \tau$ |  |  |
| 293.15 | 5.960 |  | T/298.15 |  |  |
| 293.15 | 5.679 | A | -59.7348 |  |  |
| 293.15 | 5.980 | B | 45.8700 |  |  |
| 298.15 | 5.979 | C | 46.6282 |  |  |
| 298.15 | 5.866 |  |  |  |  |
| 298.15 | 6.003 |  | $\mathrm{l}^{-1}$ ) |  |  |
| 303.15 | 6.190 |  |  |  |  |
| 308.15 | 6.483 |  |  |  |  |
| 308.15 | 6.016 |  |  |  |  |
| 313.15 | 6.546 |  |  |  |  |
| 313.15 | 6.483 |  |  |  |  |
| 313.15 | 6.795 |  |  |  |  |



FIGURE 2.1.1.2.8.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,2-cisdimethylcyclohexane.


FIGURE 2.1.1.2.8.2 Logarithm of Henry's law constant versus reciprocal temperature for 1,2-cis-dimethylcyclohexane.

TABLE 2.1.1.2.8.2
Reported vapor pressures of 1,2-cis-dimethylcyclohexane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) | $\ln \mathrm{P}=\mathrm{A})$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |
| $\ln \left(\mathrm{P} / \mathrm{P}_{\text {ref }}\right)=\left[1-\left(\mathrm{T}_{\text {ref }} / \mathrm{T}\right)\right] \cdot \exp \left(\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\right)$ | (5) |  |

Willingham et al. 1945
Stull 1947
Zwolinski \& Wilhoit 1971

| ebulliometry |  | summary of literature data |  | selected values |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 49.185 | 6352 | -15.9 | 133.3 | 18.4 | 1333 |
| 53.413 | 7655 | 7.30 | 666.6 | 31.1 | 2666 |
| 57.094 | 8966 | 18.4 | 1333 | 39.24 | 4000 |
| 60.429 | 10304 | 31.1 | 2666 | 45.33 | 5333 |
| 63.543 | 11696 | 45.3 | 5333 | 50.257 | 6666 |
| 67.742 | 13820 | 54.4 | 7999 | 54.421 | 7999 |
| 72.553 | 16608 | 66.8 | 13332 | 61.264 | 10666 |
| 77.402 | 19924 | 85.6 | 26664 | 66.815 | 13332 |
| 81.921 | 23451 | 107.0 | 53329 | 77.493 | 19998 |
| 87.974 | 28955 | 129.7 | 101325 | 85.572 | 26664 |
| 93.548 | 34897 |  |  | 92.151 | 33331 |
| 100.258 | 43324 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -50 | 97.744 | 39997 |
| 107.192 | 53656 |  |  | 106.944 | 53329 |
| 114.600 | 66759 |  |  | 114.554 | 66661 |
| 122.639 | 83718 |  |  | 120.998 | 79993 |
| 128.315 | 97607 |  |  | 126.647 | 93326 |
| 128.926 | 99203 |  |  | 127.699 | 95992 |
| 129.491 | 100694 |  |  | 128.729 | 98659 |
| 130.125 | 102389 |  |  | 129.738 | 101325 |

(Continued)

TABLE 2.1.1.2.8.2 (Continued)

| Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | summary of literature data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 130.684 | 103909 |  |  | 25.0 | 1933 |
| bp/ ${ }^{\circ} \mathrm{C}$ | 124.450 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  | A | 6.83746 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | B | 1367.311 |
| A | 6.83866 |  |  | C | 215.835 |
| B | 1345.859 |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 129.738 |
| C | 215.598 |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ |  |
| temp range $45.2-125.4{ }^{\circ} \mathrm{C}$ |  |  |  | a $25^{\circ} \mathrm{C}$ | 39.71 |
| pressure range $48-780 \mathrm{mmHg}$ |  |  |  | a bp | 33.64 |



FIGURE 2.1.1.2.8.3 Logarithm of vapor pressure versus reciprocal temperature for 1,2-cis-dimethylcyclohexane.

### 2.1.1.2.9 <br> 1,4-trans-Dimethylcyclohexane



Common Name: 1,4-trans-Dimethylcyclohexane
Synonym: trans-1,4-dimethylcyclohexane
Chemical Name: 1,4-trans-dimethylcyclohexane
CAS Registry No: 2207-04-7
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16}$
Molecular Weight: 112.213
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-36.93 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 119.4 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7626,0.7584 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 147.2, $148 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $38.14,33.05\left(25^{\circ}\right.$, bp, Dreisbach 1955)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 11.422 (Dreisbach 1955) 12.34 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
52.26, 50.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
3.84 (shake flask-GC, Price 1976; quoted, Shaw 1989)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.82180-1332.613 /\left(218.791+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $40.3-120.3^{\circ} \mathrm{C}$ (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
3025 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82180-1332.613 /\left(218.791+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $30-155^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
3026 (interpolated-Antoine eq., temp range $10.1-146.8^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81773-1330.437 /\left(218.581+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10.1-146.8^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8951.2 /(\mathrm{T} / \mathrm{K})]+7.898079$; temp range -24.3 to $119.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{atm})=[1-396.346 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.827486-6.12608 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+4.53086 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 252.05-424.25 K (Cox eq., Chao et al. 1983)

3024 (interpolated-Antoine eq., temp range $10-147^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.81773-1330.437 /\left(218.58+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10-147^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.94449-1331.612 /(-54.43+\mathrm{T} / \mathrm{K})$; temp range $313-395 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=32.5731-2.9872 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.6494 \cdot \log (\mathrm{~T} / \mathrm{K})-2.1355 \times 10^{-9} \cdot(\mathrm{~T} / \mathrm{K})+2.2946 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $236-590 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
88200 (calculated-P/C, Mackay \& Shiu 1981)
88360 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oC}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

### 2.1.1.2.10

## 1,1,3-Trimethylcyclohexane



Common Name: 1,1,3-Trimethylcyclohexane
Synonym:
Chemical Name: 1,1,3-trimethylcyclohexane
CAS Registry No: 3073-66-3
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{18}$
Molecular Weight: 126.239
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ :
-65.7 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
136.6 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.7664
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$164.7\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Ruelle \& Kesselring 1997)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
1.77 (shake flask-GC, Price 1976)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{mmHg})=6.83705-1393.299 /\left(215.551+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $54.7-137.6^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{atm})=[1-409.802 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.838270-6.63916 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+5.61172 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$
327.82-410.80 K (Cox eq., Chao et al. 1983)

1480 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.96492-1395.206 /\left(215.77+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $54.67-137.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.96816-1397.161 /\left(215.961+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $54.69-137.65^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Pasek \& Thodos 1962, Boublik et al. 1984)
1480 (interpolated-Antoine eq., temp range $55-137^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83951-1394.88 /\left(215.73+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $55-137^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.96449-1395.396 /(-57.308+\mathrm{T} / \mathrm{K})$; temp range $348-411 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
105600 (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=8.73 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=8.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

### 2.1.1.2.11 Ethylcyclohexane



Common Name: Ethylcyclohexane
Synonym:
Chemical Name: ethylcyclohexane
CAS Registry No: 1678-91-7
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16}, \mathrm{C}_{2} \mathrm{H}_{5} \mathrm{C}_{6} \mathrm{H}_{11}$
Molecular Weight: 112.213
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-111.3 (Weast 1982-83; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 131.9 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ): $0.7880 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-82)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$142.4\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Sublimation, $\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 1.0

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$7.0^{*} \quad\left(40^{\circ} \mathrm{C}\right.$, shake flask-solid phase extraction-GC, measured range $38.35-280^{\circ} \mathrm{C}$, Heidman et al. 1985) $\ln x=-334.2468+14105.21 /(\mathrm{T} / \mathrm{K})+47.93102 \cdot \ln (\mathrm{~T} / \mathrm{K})$; measured range $40-280^{\circ} \mathrm{C}$ (shake flask-solid phased extraction-GC, Heidman et al. 1985)
$7.0^{*} \quad\left(40^{\circ} \mathrm{C}\right.$, IUPAC tentative value, temp range $40-280^{\circ} \mathrm{C}$, Shaw 1989a)
3.89* (generator column-GC/FID, measured range 273.15-313.15 K, Dohányosová et al. 2004)
$\ln x=-53.6687+39.4055 / \tau+41.1210 \cdot \ln \tau, \tau=[(\mathrm{T} / \mathrm{K}) / 298.15]$, temp range $273.15-313.15 \mathrm{~K}$ (generator column-
GC/FID, Dohányosová et al. 2004)
4.36* $\quad\left(30.3^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $30.3-170.8^{\circ} \mathrm{C}$, Marche et al. 2004)
$\ln x=-344.02468+14105.21 /(\mathrm{T} / \mathrm{K})+47.93102 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $30.3-170.8^{\circ} \mathrm{C}$ (Marche et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$6351^{*} \quad\left(51.412^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $51.4-132.7^{\circ} \mathrm{C}$, Willingham et al. 1945)
1612 (extrapolated-Antoine eq., Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87041-1384.036 /\left(214.128+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $51.4-132.7^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Willingham et al. 1945)
$1333^{*} \quad\left(20.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -14.5 to $131.9^{\circ} \mathrm{C}$, Stull 1947)
1705* (extrapolated-Antoine eq., temp range $20.6-159.5^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86728-1382.466 /\left(214.995+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20.6-159.5^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99043-1381.396 /(-58.271+\mathrm{T} / \mathrm{K})$; temp range $323-407 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{MPa}\right)=325.570-18496.5 /(\mathrm{T} / \mathrm{K})-10.9666 \cdot(\mathrm{~T} / \mathrm{K})^{2}-44.7690 \cdot \ln (\mathrm{~T} / \mathrm{K}) ;$ maximum $\mathrm{k}_{\mathrm{H}}=1.186 \times 10^{4} \mathrm{MPa}$ at 385.2 K (Heidman et al. 1985)
48960* (derived from solute fugacity and mole fraction solubility, temp range 273.15-323.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 2.1.1.2.11.1
Reported aqueous solubilities of ethylcyclohexane at various temperatures

$$
\begin{equation*}
\ln x=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})+\mathrm{C} \ln (\mathrm{~T} / \mathrm{K}) \tag{1}
\end{equation*}
$$

| Heidman et al. 1985 |  | Shaw 1989a |  | Dohányosová et al. 2004 |  | Marche et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | IUPAC "tentative" best |  | generator column-GC |  | shake flask-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S / g} \cdot \mathbf{m}^{\mathbf{- 3}}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathbf{m}^{\mathbf{- 3}}$ | T/K | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{\mathbf{- 3}}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 38.35 | 6.8 | 40 | 7.0 | 274.15 | 3.803 | 30.3 | 4.358 |
| 94.45 | 15.0 | 50 | 7.0 | 274.15 | 4.108 | 70.4 | 8.790 |
| 150.25 | 120 | 60 | 7.0 | 278.15 | 3.996 | 100.5 | 28.18 |
| 206.35 | 750 | 70 | 10 | 278.15 | 3.678 | 131.0 | 67.95 |
| 263.15 | 7300 | 80 | 13 | 283.15 | 3.734 | 151.2 | 110.8 |
| 279.65 | 14600 | 90 | 16 | 288.15 | 3.759 | 170.8 | 183.3 |
|  |  | 100 | 21 | 288.15 | 3.666 |  |  |
| eq. 1 | $x$ | 120 | 55 | 293.15 | 3.766 |  |  |
| A | -334.2468 | 140 | 95 | 293.15 | 3.797 |  |  |
| B | 14105.21 | 160 | 160 | 298.15 | 3.965 |  |  |
| C | 47.93102 | 180 | 280 | 303.15 | 3.971 |  |  |
|  |  | 200 | 550 | 303.15 | 4.034 |  |  |
|  |  | 220 | 1600 | 313.15 | 4.358 |  |  |
|  |  | 240 | 3400 | 313.15 | 4.520 |  |  |
|  |  | 260 | 6500 | 313.15 | 4.364 |  |  |
|  |  | 280 | 15000 |  |  |  |  |
|  |  |  |  |  | eq. |  |  |
|  |  |  |  | $\ln x=\mathrm{A}$ | $\tau+\mathrm{C} \ln \tau$ |  |  |
|  |  |  |  |  | 298.15 |  |  |
|  |  |  |  | A | -53.6887 |  |  |
|  |  |  |  | B | 39.4055 |  |  |
|  |  |  |  | C | 41.1210 |  |  |



FIGURE 2.1.1.2.11.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for ethylcyclohexane.

TABLE 2.1.1.2.11.2
Reported vapor pressures and Henry's law constants of ethylcyclohexane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
(3a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| Vapor pressure |  |  |  |  |  | Henry's law constant <br> Dohányosová et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |  |  |
| Ebulliometry |  | Summary of literature data |  | Selected values |  | From solute fugacity $f$ and $x$ |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{H / ( P a ~ m}{ }^{\mathbf{~ m o l}}{ }^{-1}$ ) |
| 51.412 | 6351 | -14.5 | 133.3 | 20.6 | 1333 | 0 | 10422 |
| 55.636 | 7653 | 9.2 | 666.6 | 33.4 | 2666 | 5 | 14994 |
| 59.315 | 8959 | 20.6 | 1333 | 41.48 | 4000 | 10 | 20880 |
| 62.655 | 10299 | 33.4 | 2666 | 47.57 | 5333 | 15 | 28440 |
| 65.755 | 11691 | 47.6 | 5333 | 51.494 | 6666 | 20 | 37800 |
| 69.948 | 13818 | 56.7 | 7999 | 56.656 | 7999 | 25 | 48960 |
| 74.738 | 16615 | 69.0 | 13332 | 63.493 | 10666 | 30 | 62100 |
| 79.587 | 19916 | 87.8 | 26664 | 69.093 | 13332 | 35 | 77040 |
| 84.115 | 23451 | 109.1 | 53329 | 79.699 | 19998 | 40 | 93780 |
| 90.158 | 28956 | 131.8 | 101325 | 87.762 | 26664 |  |  |
| 95.716 | 34893 |  |  | 94.327 | 33331 |  |  |
| 102.412 | 43320 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -111.3 | 99.906 | 39997 |  |  |
| 109.327 | 53657 |  |  | 109.13 | 53329 |  |  |
| 116.709 | 66760 |  |  | 116.666 | 66661 |  |  |
| 124.723 | 83722 |  |  | 123.088 | 79993 |  |  |
| 130.379 | 97609 |  |  | 128.715 | 93326 |  |  |

TABLE 2.1.1.2.11.2 (Continued)

| Vapor pressure |  |  |  |  |  | Henry's law constant |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Willingham et al. 1945 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  | Dohán | sová et al. 2004 |
| Ebulliometry |  | Summary of literature data |  | Selected values |  | From solute fugacity $f$ and $x$ |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} \mathrm{~mol}^{-1}$ ) |
| 130.988 | 99208 |  |  | 129.764 | 95992 |  |  |
| 131.551 | 100700 |  |  | 130.79 | 98659 |  |  |
| 132.181 | 102404 |  |  | 131.795 | 101325 |  |  |
| 132.742 | 103922 |  |  | 25.0 | 1707 |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 131.783 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
| Antoine eq. |  |  |  | A | 6.86728 |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | B | 1382.466 |  |  |
| A | 6.87041 |  |  | C | 214.995 |  |  |
| B | 1384.036 |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 131.795 |  |  |
| C | 214.128 |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ |  |  |  |
| temp range $51.4-132.7^{\circ} \mathrm{C}$ |  |  |  | at $25^{\circ} \mathrm{C}$ | 40.48 |  |  |
| pressure range $48-780 \mathrm{mmHg}$ |  |  |  | at bp | 34.31 |  |  |



FIGURE 2.1.1.2.11.2 Logarithm of vapor pressure versus reciprocal temperature for ethylcyclohexane.


FIGURE 2.1.1.2.11.3 Logarithm of Henry's law constant versus reciprocal temperature for ethylcyclohexane.

### 2.1.1.2.12



Common Name: Cycloheptane
Synonym: suberane
Chemical Name: cycloheptane
CAS Registry No: 291-64-5
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{14}$
Molecular Weight: 98.186
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -12 -8.46 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right): 118.5$ 118.4 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ : $0.8098 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1984) 0.80656 (measured, Anand et al. 1975)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $121.3\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987) 136.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $4.98,0.29,0.45,1.88\left(-138.35,-74.95,-60.75,-8.05^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
47.6, 48.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
30.0 (shake flask-GC, McAuliffe 1966)
$27.1 \quad\left(30^{\circ} \mathrm{C}\right.$, shake flask-GC, Groves 1988)
23.5, $23.5 \quad\left(25,30^{\circ} \mathrm{C}\right.$, calculated-liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
19920* $\quad\left(68.2^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $68.2-159^{\circ} \mathrm{C}$, Finke et al. 1956)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85271-1330.742 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+216.246\right)$; temp range $68.2-159^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Finke et al. 1956)
2924* (static method-quartz spiral gauge, measured range 283.048-323.551 K, Anand et al. 1975)
$\log (\mathrm{P} / \mathrm{kPa})=6.19317-1450.17 /(\mathrm{T} / \mathrm{K}-44.91)$; temp range $283.048-323.551 \mathrm{~K}$ (static method, vapor-liquid equilibria study, Anand et al. 1975)
$16312^{*} \quad\left(63.03^{\circ} \mathrm{C}\right.$, comparative ebulliometry, measured range $60-121.7^{\circ} \mathrm{C}$, Meyer \& Hotz 1976)
$\log (\mathrm{P} / \mathrm{mmHg})=5.85683-1333.780 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+216.6438\right)$; temp range $60-121.7^{\circ} \mathrm{C}$ (Antoine eq., comparative ebulliometry, Meyer \& Hotz 1976)
$\log (\mathrm{P} / \mathrm{atm})=[1-391.896 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.885524-8.19621 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+7.88065 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 284.35-432.17 K (Cox eq., Chao et al. 1983)

2895, 2898 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.97858-1331.383 /\left(214.325+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $60.2-159^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.98198-1333.899 /\left(216.657+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $63.03-121.68^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
2895 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85395-1331.57 /\left(216.35+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $68-159^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
2930 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.98143-1333.833 /(-56.458+\mathrm{T} / \mathrm{K})$; temp range $341-433 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.12682-1417.738 /(-47.665+\mathrm{T} / \mathrm{K})$; temp range $282-333 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.97596-1329.98 /(-56.968+\mathrm{T} / \mathrm{K})$; temp range $333-398 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.05325-2475.271 /(108.392+\mathrm{T} / \mathrm{K})$; temp range $476-604 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=54.0858-3.6109 \times 10^{3} /(\mathrm{T} / \mathrm{K})-17.331 \cdot \log (\mathrm{~T} / \mathrm{K})+7.5292 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.7553 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $265-604 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
9977 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.87 (calculated $-\pi$ substituent constant, Hansch et al. 1968)
3.06 (calculated-MCI $\chi$, Murray et al. 1975)
3.76 (calculated-fragment const., Yalkowsky \& Morozowich 1980)
2.72 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.91 (calculated-fragment const., Müller \& Klein 1992)
3.1648 (calculated-UNIFAC group contribution, Chen et al. 1993)
4.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, * data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=13.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=(7.88 \pm 1.38) \times 10^{12} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 298 K (flash photolysis-resonance absorption, Jolly et al. 1985)
$\mathrm{k}_{\mathrm{OH}}=(11.8-13.1) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298-300 \mathrm{~K}$ (review, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=1.25 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=13.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.12.1
Reported vapor pressures of cycloheptane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(2)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ |  | (4) |
| $\log \mathrm{P}=\mathrm{A}^{\prime}\left[1-\left(\mathrm{T}_{\mathrm{B}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right]$ |  | (5) where $\mathrm{A}^{\prime}=\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}$ |



| Cox eq. |  |
| :--- | :---: |
| eq. 5 | P/atm |
| $\mathrm{T}_{\mathrm{B}}$ | 391.953 |
| a | 0.839608 |
| - b $\times 10^{4}$ | 6.9133 |
| $\mathrm{c} \times 10^{7}$ | 6.4035 |



FIGURE 2.1.1.2.12.1 Logarithm of vapor pressure versus reciprocal temperature for cycloheptane.

### 2.1.1.2.13



Common Name: Cyclooctane Synonym:
Chemical Name: cyclooctane
CAS Registry No: 292-64-8
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16}$
Molecular Weight: 112.213
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ : 14.59 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right): 151$ 149 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.8340 \quad$ (Weast 1984)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $134.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987) 154.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 6.32, 0.48, $2.41\left(-106.65,-89.35,14.85^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
48.89, 51.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
7.90 (shake flask-GC, McAuliffe 1966)
7.48 (calculated-recommended liquid-liquid equilibrium LLE data, Ma̧czyński et al. 2004)
5.80* (generator column-GC, measured range 27.15-313.15 K, Dohányosová et al. 2004)
$\ln x=-55.1375+41.2528 / \tau+43.2804 \cdot \ln \tau ; \tau=\mathrm{T} / 298.15 \mathrm{~K}$ (empirical eq., generator column-GC, Dohányosová et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
19920* ( $96.7^{\circ} \mathrm{C}$, ebulliometry, measured range $96.7-194.4^{\circ} \mathrm{C}$, Finke et al. 1956)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86173-1437.682 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+210.003\right)$; temp range $96.7-194.4^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Finke et al. 1956)
748* (static-quartz spiral gauge, measured range 290.961-323.326 K, Anand et al. 1975)
$\log (\mathrm{P} / \mathrm{kPa})=5.97188-1447.45 /(\mathrm{T} / \mathrm{K}-60.67)$; temp range $291-323 \mathrm{~K}$ (static method, vapor-liquid equilibria VLE study, Anand et al. 1975)
22454* (100.133 ${ }^{\circ} \mathrm{C}$, comparative ebulliometry, measured range $100.1-161^{\circ} \mathrm{C}$, Meyer \& Hotz 1976)
$\log (\mathrm{P} / \mathrm{mmHg})=5.861786-1438.455 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+210.1844\right)$; temp range $100.1-161^{\circ} \mathrm{C}$ (Antoine eq., comparative ebulliometry, Meyer \& Hotz 1976)
767, 740 (extrapolated-Antoine eq., extrapolated, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.98693-1437.751 /\left(210.012+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $96.7-194.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.06524-1492.101 /\left(216.413+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $100.1-160.9^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
740 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86187-1437.79 /\left(210.02+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $97-194^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$ 753 (interpolated-Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.98663-1437.682 /(-63.147+\mathrm{T} / \mathrm{K})$; temp range $369-487 \mathrm{~K}$ (Antoine eq. -I , Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.9899-1440.707 /(-62.701+\mathrm{T} / \mathrm{K})$; temp range $369-468 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.20474-1564.985 /(-50.842+\mathrm{T} / \mathrm{K})$; temp range $289-369 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
10485 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
14526* (derived from solute fugacity and mole fraction solubility, temp range 273.15-313.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
3.28 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
3.50 (calculated-MCI $\chi$, Murray et al. 1975)
3.28 (Hutchinson et al. 1980; Sangster 1989)
3.28 (calculated-fragment const., Lyman 1982)
4.45 (recommended, Sangster 1989)
3.04 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
4.47 (calculated-fragment const., Müller \& Klein 1992)
3.6117 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference: $\mathrm{k}_{\mathrm{OH}}=14.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997) Oxidation:
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$ for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

TABLE 2.1.1.2.13.1
Reported aqueous solubilities and Henry's law constants of cyclooctane at various temperatures

| Aqueous solubility |  |  |  | Henry's law constant |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Dohányosová et al. 2004 |  |  |  | Dohányosová et al. 2004 |  |
| generator column-GC |  | smoothed exptl raw data |  | from solute fugacity $f$ and $x$ |  |
| T/K | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) |
|  | raw data |  |  |  |  |
| 274.15 | 5.53 | 273.15 | 5.73 | 273.15 | 2826 |
| 274.15 | 5.885 | 278.15 | 5.59 | 278.15 | 4158 |
| 278.15 | 5.548 | 283.15 | 5.53 | 283.15 | 5922 |
| 278.15 | 5.442 | 288.15 | 5.55 | 288.15 | 8190 |
| 283.15 | 5.548 | 293.15 | 5.64 | 293.15 | 11052 |
| 288.15 | 5.754 | 298.15 | 5.80 | 298.15 | 14526 |
| 293.15 | 5.492 | 303.15 | 6.02 | 303.15 | 18720 |
| 298.15 | 5.848 | 308.15 | 6.32 | 308.15 | 23400 |
| 298.15 | 5.530 | 313.15 | 6.68 | 313.15 | 28800 |
| 303.15 | 5.922 |  |  |  |  |
| 303.15 | 5.835 | $\ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau$ |  |  |  |
| 308.15 | 6.483 | $\tau=\mathrm{T} / 298.15$ |  |  |  |
| 308.15 | 6.421 | A | -55.1375 |  |  |
| 313.15 | 6.733 | B | 41.2528 |  |  |
| 313.15 | 6.858 | C | 43.2804 |  |  |



FIGURE 2.1.1.2.13.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for cyclooctane.


FIGURE 2.1.1.2.13.2 Logarithm of Henry's law constant versus reciprocal temperature for cyclooctane.

TABLE 2.1.1.2.13.2
Reported vapor pressures of cyclooctane at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}^{\prime}\left[1-\left(\mathrm{T}_{\mathrm{B}} / \mathrm{K}\right) /(\mathrm{T} / \mathrm{K})\right]$
(5) where $\mathrm{A}^{\prime}=\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}$

| Finke et al. 1956 |  | Anand et al. 1975 |  | Meyer \& Hotz 1976 |  | Dohányosová et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | static-quartz spiral gauge |  | comparative ebulliometry |  | from Anand et al. 1975 |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa | $t^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | T/K | P/Pa |
| 96.711 | 19920 | 290.961 | 488 | 100.133 | 22454 | 273.15 | 207 |
| 103.318 | 25007 | 294.376 | 601 | 108.375 | 29598 | 278.15 | 292 |
| 109.977 | 31160 | 298.150 | 748 | 118.813 | 41155 | 283.15 | 406 |
| 116.694 | 38457 | 302.060 | 944 | 127.569 | 53410 | 288.15 | 557 |
| 123.472 | 47359 | 306.922 | 1244 | 139.435 | 74511 | 293.15 | 753 |
| 130.301 | 70109 | 311.678 | 1605 | 149.031 | 95919 | 303.15 | 1010 |
| 137.190 | 84525 | 316.472 | 2056 | 157.388 | 118293 | 308.15 | 1330 |
| 144.133 | 101325 | 323.326 | 2890 | 160.911 | 129263 | 313.15 | 1730 |
| 151.146 | 120798 |  |  |  |  |  |  |
| 158.203 | 143268 | Antoine eq. |  | bp/ ${ }^{\circ} \mathrm{C}$ | 151.148 |  |  |
| 165.321 | 169052 | eq. 3 | P/kPa | Antoine eq. |  |  |  |
| 172.502 | 198530 | A | 6.91788 | eq. 2 | $\mathrm{P} / \mathrm{cmHg}$ |  |  |
| 187.040 | 232087 | B | 1447.45 | A | 5.861786 |  |  |
| 194.397 | 270110 | C | -60.67 | B | 1438.455 |  |  |
|  |  |  |  | C | 210.1844 |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 151.14 |  |  | temp range $100-161^{\circ} \mathrm{C}$ |  |  |  |
| $\begin{aligned} & \text { Antoine eq. } \\ & \text { eq. } 2\end{aligned} \quad \mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |  |  |  |
|  |  |  |  | Cox equation: |  |  |  |

TABLE 2.1.1.2.13.2 (Continued)

| Finke et al. 1956 |  | Anand et al. 1975 |  | Meyer \& Hotz 1976 |  | Dohányosová et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | static-quartz spiral gauge |  | comparative ebulliometry |  | from Anand et al. 1975 |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| A | 686173 |  |  | eq 5 | P/atm |  |  |
| B | 1437.682 |  |  |  | 0.869777 |  |  |
| C | 210.003 |  |  | $\begin{gathered} -b \times 10^{3} \\ c \times 10^{6} \end{gathered}$ | $\begin{aligned} & 0.775348 \\ & 0.716695 \end{aligned}$ |  |  |
| Cox equation: |  |  |  |  |  |  |  |
| eq 5 | P/atm |  |  |  |  |  |  |
| a | 0.839609 |  |  |  |  |  |  |
| $-\mathrm{b} \times 10^{4}$ | 6.2033 |  |  |  |  |  |  |
| $\mathrm{c} \times 10^{7}$ | 5.177 |  |  |  |  |  |  |
| $\mathrm{T}_{\text {B }}$ | 424.300 |  |  |  |  |  |  |



FIGURE 2.1.1.2.13.3 Logarithm of vapor pressure versus reciprocal temperature for cyclooctane.

### 2.1.1.2.14

Decalin


Common Name: Decalin
Synonym: bicyclo[4.4.0]decane, naphthalane, naphthane
Chemical Name: decahydronaphthalene (mixed isomers)
CAS Registry No: 91-17-8
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{18}$
Molecular Weight: 138.250
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-42.9 (cis-decalin, Lide 2003)
-30.4 (trans-decalin, Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right): 191.7$
195.774 (cis-decalin, Camin \& Rossini 1955)
187.273 (trans-decalin, Camin \& Rossini 1955)
191.7 (Riddick et al. 1986)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.8865,0.8789 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, mixed isomers, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
154.8, 159.6 (cis-decalin, trans-decalin, calculated-density, Stephenson \& Malanowski 1987)
184.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
41.09 (bp, mixed isomers, Riddick et al. 1986)
51.342, $40.999 \quad$ (cis-decalin, $25^{\circ} \mathrm{C}$, bp, Riddick et al. 1986)
49.87, $40.229 \quad$ (trans-decalin, $25^{\circ} \mathrm{C}$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
14.414, 9.489 (cis-decalin, trans-decalin, Riddick et al. 1986)
14.43 (cis-decalin, Chickos et al. 1999)

2,13, 9.49 (trans-decalin, $-57.05,42.95^{\circ} \mathrm{C}$, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
59.45, 52.1 (cis-decalin: exptl., calculated-group additivity method, Chickos et al. 1999)
51.1, 52.1 (trans-decalin: exptl, calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.889 (shake flask-GC, Price 1976; quoted as more reliable value, Shaw 1989)
6.21 (shake flask-GC, Hutchinson et al. 1980)
1.99 (calculated-QSAR, Passino \& Smith 1987)
2.14 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
133.3* $\quad\left(23.3^{\circ} \mathrm{C}\right.$, isomer not specified, ebulliometry, measured range 23.3-150.0 ${ }^{\circ} \mathrm{C}$, Gardner \& Brewer 1937)
$241^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, cis-decalin, manometry, measured range -29.5 to $194.7^{\circ} \mathrm{C}$, Seyer \& Mann 1945)
$381^{*} \quad\left(13^{\circ} \mathrm{C}\right.$, trans-decalin, manometry, measured range -30.0 to $235.3^{\circ} \mathrm{C}$, Seyer \& Mann 1945)
$133.3^{*} \quad\left(22.5^{\circ} \mathrm{C}\right.$, cis-decalin, summary of literature data, temp range $22.5-194.6^{\circ} \mathrm{C}$, Stull 1947)
$666.6^{*} \quad\left(30.6^{\circ} \mathrm{C}\right.$, trans-decalin, summary of literature data, temp range -0.80 to $186.7^{\circ} \mathrm{C}$, Stull 1947)
$5529^{*} \quad\left(99.883^{\circ} \mathrm{C}\right.$, cis-decalin, ebulliometry, measured range $99.883-196.376^{\circ} \mathrm{C}$, Camin \& Rossini 1955)
5530* ( $92.36^{\circ} \mathrm{C}$, trans-decalin, ebulliometry, measured range $92.36-187.867^{\circ} \mathrm{C}$, Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87529-1594.460 /\left(203.392+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $99.8-196.4^{\circ} \mathrm{C}$ (cis-decalin, Antoine eq., ebulliometry-manometer measurement, Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85681-1564.683 /\left(206.259+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $92.3-187.0^{\circ} \mathrm{C}$ (trans-decalin, Antoine eq., ebulliometry-manometer measurement, Camin \& Rossini 1955)
104*, 164* (cis-decalin, trans-decalin, interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87529-1594.460 /\left(203.392+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $68.0-277.67^{\circ} \mathrm{C}$ (cis-decalin, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85681-1564.683 /\left(206.259+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $60.91-218.88^{\circ} \mathrm{C}$ (trans-decalin, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10515.4 /(\mathrm{T} / \mathrm{K})]+7.797540$; temp range $22.5-194.6^{\circ} \mathrm{C}$ (cis-decalin, Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8749.1 /(\mathrm{T} / \mathrm{K})]+6.973042$; temp range -0.80 to $186.7^{\circ} \mathrm{C}$ (trans-decalin, Antoine eq., Weast 1972-73)
$\log (\mathrm{P} /$ atm $)=[1-468.915 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.683577-0.900942 \times 10^{-4} .(\mathrm{T} / \mathrm{K})+2.28255 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range 295.65-727.59 K (cis-decalin, Cox eq., Chao et al. 1983)
$\log (\mathrm{P} / \mathrm{atm})=[1-460.458 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.880979-6.38749 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+4.59180 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 365.51-461.02 K, (trans-decalin, Cox eq., Chao et al. 1983)

178, 104 (cis-decalin, calculated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.96043-2358.398 /\left(280.79+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -29.5 to $194.7^{\circ} \mathrm{C}$ (cis-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.00042-1594.653 /\left(203.415+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $99.88-196.4^{\circ} \mathrm{C}$ (cis-decalin, Antoine eq. from reported exptl. data of Camin \& Rossini 1955, Boublik et al. 1984)
434, 165 (trans-decalin, calculated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=7.69594-3126.688 /\left(363.012+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -30.0 to $253.3^{\circ} \mathrm{C}$ (trans-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.98704-1568.642 /\left(206.726+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $92.36-187.9^{\circ} \mathrm{C}$ (trans-decalin, Antoine eq. from reported exptl. data of Camin \& Rossini 1955, Boublik et al. 1984)
104, 168 (cis-, trans-decalin, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87529-1594.81 /\left(203.39+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range $68-228^{\circ} \mathrm{C}$ (cis-decalin Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86581-1564.683 /\left(206.26+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $61-219^{\circ} \mathrm{C}$ (trans-decalin Antoine eq., Dean 1985, 1992)
130 (mixed isomer, $23.3^{\circ} \mathrm{C}$, lit. average, Riddick et al. 1986)
100, 164 (selected lit., cis-, trans-decalin, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.00019-1594.460 /\left(203.392+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range not specified (cis-decalin, Antoine eq., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.98171-1564.683 /\left(206.259+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range not specified (trans-decalin, Antoine eq., Riddick et al. 1986)
105, 168 (cis-decalin, trans-decalin, extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.00019-1595.176 /(-69.622+\mathrm{T} / \mathrm{K})$; temp range $371-473 \mathrm{~K}$ (cis-decalin, Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99363-1573.981 /(-65.77+\mathrm{T} / \mathrm{K})$; temp range $363-461 \mathrm{~K}$ (trans-decalin, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=45.6345-4.21 \times 10^{3} /(\mathrm{T} / \mathrm{K})-12.881 \cdot \log (\mathrm{~T} / \mathrm{K})-7.8083 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+2.8637 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $230-702 \mathrm{~K}$ (cis-decalin, vapor pressure eq., Yaws 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=76.1002-5.03 \times 10^{3} /(\mathrm{T} / \mathrm{K})-25.078 \cdot \log (\mathrm{~T} / \mathrm{K})+9.7608 \times 10^{-3} .(\mathrm{T} / \mathrm{K})-2.5814 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $243-687 \mathrm{~K}$ (trans-decalin, vapor pressure eq., Yaws 1994)
$128^{*} \quad\left(20.42^{\circ} \mathrm{C}\right.$, trans-decalin, differential pressure gauge, measured range -29.31 to $160.7^{\circ} \mathrm{C}$, Mokbel et al. 1995)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
11855* (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$ Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=11.85-4125 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}($ EPICS measurements, Ashworth et al. 1988)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.79 (calculated-fragment const., Müller \& Klein 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=1.96 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}$ of cis-decalin and $2.02 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ of trans-decalin at 299 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=2.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ for the reaction at 298 K (Atkinson 1990)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:

TABLE 2.1.1.2.14.1
Reported vapor pressures and Henry's law constants of decalin (isomer not specified) at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$

Vapor pressure Henry's law constant

| Gardner \& Brewer 1937 |  |  |  | Ashworth et al. 1988 <br> EPICS-GC |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  |  |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 23.3 | 133.3 | 60.0 | 987 | 10 | 7093 |
| 32.8 | 240 | 66.1 | 1293 | 15 | 8481 |
| 37.3 | 280 | 86.8 | 3520 | 20 | 10740 |
| 38.4 | 320 | 96.0 | 5186 | 25 | 11855 |
| 42.5 | 400 | 104.5 | 7293 | 30 | 20164 |
| 43.0 | 413 | 118.8 | 11652 |  |  |
| 49.6 | 587 | 133.8 | 20278 |  | - B/(T/K) |
| 50.6 | 627 | 150.0 | 31997 | eq. 4 a | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ |
| 54.3 | 747 |  |  | A | 11.85 |
| 54.6 | 800 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 193.8 | B | 4125 |
| 59.8 | 1027 |  |  |  |  |



FIGURE 2.1.1.2.14.1 Logarithm of vapor pressure versus reciprocal temperature for decalin.


FIGURE 2.1.1.2.14.2 Logarithm of Henry's law constant versus reciprocal temperature for decalin.

TABLE 2.1.1.2.14.2
Reported vapor pressures of cis-decalin at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log P=A-B /(C+T / K)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \ln (\mathrm{T} / \mathrm{K})$

Seyer \& Mann 1945
Stull 1947

| manometry |  |
| :---: | ---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| -29.5 | 51 |
| -19.2 | 87 |
| -10.0 | 115 |
| 0.0 | 145 |
| 12.0 | 196 |
| 20.0 | 241 |
| 38.0 | 457 |
| 43.4 | 532 |
| 49.9 | 704 |
| 50.4 | 719 |
| 52.9 | 805 |
| 56.9 | 971 |
| 10.0 | 1095 |
| 70.0 | 1669 |
| 80.1 | 2590 |
| 92.4 | 4358 |
| 105.1 | 7239 |
| 109.8 | 8389 |
| 112.4 | 9121 |
| 124.6 | 13976 |
| 148.7 | 29997 |
| 172.7 | 57690 |
| 194.700 | 101093 |
| eq .4 |  |
| A | $\mathrm{P} / \mathrm{cmHg}$ |
| B | 6.8139 |
| C | 1702.20 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 34.32 |
|  | 194.5 |

Camin \& Rossini 1955 Zwolinski \& Wilhoit 1971
ebulliometry
selected values

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :---: | :---: |
| 99.883 | 5529 |


| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :---: | :---: |
| 68.0 | 1333 |

105.685694

| 110.490 | 8331 |
| :--- | :--- |
| 114.152 | 9523 |

118.00410943
123.13213008
10
109.391
117.280

| 128.731 | 15827 | 117.280 |
| :--- | :--- | :--- |
| 135.021 | 19433 | 123.676 |

$140.176 \quad 22881$

| 147.456 | 28546 | 1 |
| :--- | :--- | :--- |
| 154.245 | 34817 | 1 |


| 154.245 | 34817 |
| :--- | :--- |
| 161.885 | 43164 |


| 161.885 | 43164 | 1 |
| :--- | :--- | :--- |
| 170.056 | 53773 | 169 |


| 178.629 | 53773 | 1 |
| :--- | :--- | :--- |
| 17068 |  |  |


| 187.823 | 83031 | 185.724 | 79993 |
| :--- | :--- | :--- | :--- |


| 194.370 | 98080 | 192.251 | 93326 |
| :--- | :--- | :--- | :--- |


| 195.055 | 99658 | 193.389 | 95992 |
| :--- | :--- | :--- | :--- |


| 195.635 | 101001 | 194.622 | 98659 |
| ---: | ---: | ---: | ---: |
| 196.376 | 102727 | 195.774 | 101325 |

$\mathrm{bp} /{ }^{\circ} \mathrm{C} \quad 195.774$

| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| :---: | :---: | :---: | :---: |
| A | 6.87529 | A | 6.87529 |
| B | 1594.460 | B | 1594.460 |
| C | 203.392 | C | 203.392 |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 195.774 |
|  |  | $\Delta \mathrm{H}_{\mathrm{v}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=39.30$ |  |

at bp


FIGURE 2.1.1.2.14.3 Logarithm of vapor pressure versus reciprocal temperature for cis-decalin.
TABLE 2.1.1.2.14.3
Reported vapor pressures of trans-decalin at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log P=A-B /(C+T / K)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \ln (\mathrm{T} / \mathrm{K})$
(1a)
(2a)
1.

| Seyer \& Mann 1945 |  | Stull 1947 |  | Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| manometry |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -30.0 | 59 | -0.80 | 133.3 | 92.36 | 5530 | 60.91 | 1333 |
| -24.1 | 80 | 30.6 | 666.6 | 98.129 | 6942 | 75.37 | 2666 |
| -11.1 | 143 | 47.2 | 1333 | 102.891 | 8331 | 84.59 | 4000 |
| -0.70 | 229 | 65.3 | 2666 | 106.500 | 9522 | 91.527 | 5333 |
| 0.0 | 241 | 85.7 | 5333 | 110.316 | 10946 | 97.072 | 6666 |
| 13.0 | 381 | 98.4 | 7999 | 115.356 | 13086 | 101.800 | 7999 |
| 30.9 | 801 | 114.6 | 13332 | 120.918 | 15828 | 109.599 | 10666 |
| 51.5 | 1597 | 136.2 | 26664 | 127.140 | 19434 | 115.922 | 13332 |
| 59.7 | 2221 | 160.1 | 53329 | 132.255 | 22434 | 128.045 | 19998 |
| 65.3 | 2657 | 186.7 | 101325 | 146.156 | 34817 | 137.182 | 26664 |
| 74.4 | 3562 |  |  | 153.719 | 43163 | 144.649 | 33331 |
| 83.5 | 5072 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -30.7 | 161.801 | 53773 | 150.991 | 39997 |
| 95.5 | 7307 |  |  | 170.297 | 67069 | 161.522 | 53329 |
| 112.4 | 12635 |  |  | 179.395 | 84031 | 170.018 | 66661 |
| 119.4 | 16087 |  |  | 185.885 | 98081 | 177.320 | 79993 |
| 136.7 | 27478 |  |  | 186.563 | 99665 | 183.783 | 93326 |
| 152.3 | 42595 |  |  | 187.140 | 101005 | 184.911 | 95992 |
| 168.0 | 65024 |  |  | 187.867 | 102731 | 186.132 | 98659 |

TABLE 2.1.1.2.14.3 (Continued)

| Seyer \& Mann 1945 |  | Stull 1947 |  | Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| manometry |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 187.1 | 103009 |  |  |  |  | 187.274 | 101325 |
| 209.8 | 170060 |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 187.273 |  |  |
| 212.9 | 185496 |  |  |  |  |  |  |
| 223.4 | 228787 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 235.3 | 284978 |  |  | A | 6.85681 | A | 6.83561 |
|  |  |  |  | B | 1564.683 | B | 1564.683 |
| bp/ ${ }^{\circ} \mathrm{C}$ | 185.8 |  |  | C | 206.259 | C | 206.269 |
| eq. 4 a | $\mathrm{P} / \mathrm{cmHg}$ |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 187.274 |
| A | 6.8509 |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{k}$ | $\left.{ }^{1}\right)=38.50$ |
| B | 2182.38 |  |  |  |  |  | at bp |
| C | 32.64 |  |  |  |  |  |  |

2. 

Mokbel et al. 1995

| static method-manometry |  |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| -29.31 | 1.91 | 40.37 | 448 | 99.60 | 7347 |
| -19.37 | 5.23 | 50.42 | 790 | 109.58 | 10670 |
| -9.42 | 13.2 | 60.41 | 1329 | 119.69 | 15160 |
| 0.46 | 29.4 | 64.63 | 1636 |  |  |
| 10.44 | 63.1 | 69.55 | 2050 | data fitted to Wagner eq. |  |
| 20.42 | 128 | 79.48 | 3219 |  |  |
| 30.35 | 245 | 89.54 | 4939 |  |  |



FIGURE 2.1.1.2.14.4 Logarithm of vapor pressure versus reciprocal temperature for trans-decalin.

### 2.1.2 Unsaturated Hydrocarbons

### 2.1.2.1 Alkenes

### 2.1.2.1.1 2-Methylpropene



Common Name: 2-Methylpropene
Synonym: isobutene, isobutylene
Chemical Name: 2-methylpropene
CAS Registry No: 115-11-7
Molecular Formula: $\mathrm{C}_{4} \mathrm{H}_{8} ; \mathrm{CH}_{3} \mathrm{C}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{2}$
Molecular Weight: 56.107
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-140.7 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
-6.9 (Dreisbach 1959; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.5942,0.5879 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$94.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966)
$95.4 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
88.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
5.92 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
44.72, 41.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
263 (shake flask-GC, of liquid at 1 atmospheric pressure, McAuliffe 1966)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
$131695^{*}, 131855\left(0^{\circ} \mathrm{C}\right.$, static method-manometer, measured range -56.75 to $0^{\circ} \mathrm{C}$, Lamb \& Roper 1940)
$101325^{*} \quad\left(-6.9^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -105.1 to $-6.9^{\circ} \mathrm{C}$, Stull 1947)
303700 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84134-923.2 /\left(240.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -68 to $39^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

302642* (extrapolated-Antoine eq., temp range -81.95 to $11.88^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84134-923.200 /\left(240.00+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -81.95 to $11.88^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 5742.9 /(\mathrm{T} / \mathrm{K})]+7.601563$; temp range -105.1 to $-6.90^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=6.68466-886.25 /\left(234.64+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -82 to $12^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
303255 (interpolated-Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.96624-923.2 /(-33.15+\mathrm{T} / \mathrm{K})$; temp range $212-279 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93211-907.644 /(-35.082+\mathrm{T} / \mathrm{K})$; temp range $266-313 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.27428-1095.288 /(-9.441+\mathrm{T} / \mathrm{K})$; temp range 310-376 K (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.64267-2336.466 /(160.311+\mathrm{T} / \mathrm{K})$; temp range $371-418 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=39.2295-2.1094 \times 10^{3} /(\mathrm{T} / \mathrm{K})-12.567 \cdot \log (\mathrm{~T} / \mathrm{K})+7.7304 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-1.3659 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $133-418 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$607940\left(45.44^{\circ} \mathrm{C}\right.$, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
$21600 \quad$ (calculated $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
23100, 10800 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
14800 (calculated-P/C, Mackay \& Shiu 1981)
$35800 \quad$ (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
20994 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
$0.64,1.32$ (quoted, calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, * data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}=6.2 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Hanst et al. 1958)
$\mathrm{k}_{\mathrm{O} 3}=2.32 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $30^{\circ} \mathrm{C}$ (flow system, Bufalini \& Altshuller 1965)
$\mathrm{k}_{\mathrm{OH}}=6.46 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (discharge flow system-MS, Morris \& Niki 1971)
$\mathrm{k}_{\mathrm{O} 3}=13.6 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \cdot \mathrm{~s}^{-1}$ at room temp (Japar et al. 1974)
$\mathrm{k}_{\mathrm{O} 3}=11.7 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Huie \& Herron 1975)
$\mathrm{k}_{\mathrm{OH}}=(3.05 \pm 0.31) \times 10^{10} \mathrm{~cm}^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Winer et al. 1976)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.60 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atoms (Singleton \& Cvetanovic 1976; Atkinson \& Pitts Jr. 1977; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}} *=5.07 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297.2 K , measured range $297-425 \mathrm{~K}$ (flash photolysis-resonance fluorescence, Atkinson \& Pitts 1977)
$\mathrm{k}_{\mathrm{O} 3}=11.7 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (chemiluminescence, Adeniji et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=5.13 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=(6.46 \pm 0.13) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1984)
$\mathrm{k}_{\mathrm{O} 3}=5.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=5.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O} 3}=1.21 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (review, Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=5.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=31.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=(3.15-3.38) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}} *=5.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=3.32 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3} *=11.3 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.69 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: atmospheric lifetime was estimated to be 5.3 h , based on photooxidation rate constant $\mathrm{k}=5.14 \times 10^{-11}$ $\mathrm{cm}^{3}$. molecule ${ }^{-1} \mathrm{~s}^{-1}$ with OH radicals in air during summer daylight (Altshuller 1991).

Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins and $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$ for substituted olefins, based on rate constant $\mathrm{k}=1 \times 10^{6} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation by singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.1.1
Reported vapor pressures of 2-methylpropene (isobutene) at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})$
(5)

| Lamb \& Roper 1940 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static method-manometer |  | summary of literature data |  | selected values |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -56.75 | 8725 | -105.1 | 133.3 | -81.95 | 1333 | -8.983 | 93326 |
| -25.30 | 47703 | -96.5 | 666.6 | -73.37 | 2666 | -8.274 | 95992 |
| -20.88 | 57462 | -81.9 | 1333 | -67.90 | 4000 | -7.580 | 98659 |
| -7.47 | 99791 | -73.4 | 2666 | -63.79 | 5333 | -6.900 | 101325 |
| -0.67 | 128789 | -63.8 | 5333 | -60.472 | 6666 | 25.0 | 302642 |
| 0.0 | 131695 | -57.7 | 7999 | -57.664 | 7999 |  |  |
| 0.0 | 131855 | -49.3 | 13332 | -53.051 | 10666 |  |  |
|  |  | -36.7 | 26664 | -49.309 | 13332 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| bp/ ${ }^{\circ} \mathrm{C}$ | -7.12 | -22.2 | 53329 | -42.111 | 19998 | A | 6.84134 |
| eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | -6.9 | 101325 | -36.666 | 26664 | B | 923.200 |
| A | 9.77465 |  |  | -32.231 | 33331 | C | 240.000 |
| B | 1503.866 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -140.3 | -28.462 | 39997 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | -6.90 |
| C | 0.0046649 |  |  | -22.227 | 53329 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ} \mathrm{m}$ |  |
|  |  |  |  | -17.133 | 66661 | at $25^{\circ} \mathrm{C}$ | 20.59 |
|  |  |  |  | -12.789 | 79993 | at bp | 22.12 |



FIGURE 2.1.2.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpropene.

### 2.1.2.1.2 1-Butene



Common Name: 1-Butene
Synonym: butylene
Chemical Name: 1-butene
CAS Registry No: 106-98-9
Molecular Formula: $\mathrm{C}_{4} \mathrm{H}_{8} ; \mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{CHCH}_{2}$
Molecular Weight: 56.107
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -185.34 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : -6.26 (Dreisbach 1959; Stephenson \& Malanowski 1987; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.5951,0.5888\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, at saturation pressure, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $94.3\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Ruelle \& Kesselring 1997)
$95.3 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
88.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
3.85 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
43.84, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
222 (shake flask-GC, liquid at 1 atmospheric pressure, McAuliffe 1966)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$128536^{*} \quad\left(0^{\circ} \mathrm{C}\right.$, static method-manometer, measured range -56.75 to $0^{\circ} \mathrm{C}$, Lamb \& Roper 1940)
$\log (\mathrm{P} / \mathrm{mmHg})=-1330.977 /(\mathrm{T} / \mathrm{K})-0.0017607 \cdot(\mathrm{~T} / \mathrm{K})+8.33816$; temp range $195-274 \mathrm{~K}$ (static method, Lamb \& Roper 1940)
361100* (Antoine eq. regression, temp range -104.8 to $-6.3^{\circ} \mathrm{C}$, Stull 1947)
296000 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84290-926.1 /\left(240.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -67 to $40^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959) 297309* (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84290-926.10 /\left(240.00+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -81.5 to $12.6^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 5996.7 /(\mathrm{T} / \mathrm{K})]+7.826754$; temp range -104.8 to $-6.3^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=6.531-810.261 /\left(228.066+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ (Antoine eq. from reported exptl. data, Boublik et al. 1984) $\log (\mathrm{P} / \mathrm{mmHg})=6.79290-908.80 /\left(238.54+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -82 to $13^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
297020, 295800 (interpolated-Antoine eq.-III, V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.9678-926.1 /(-33.15+\mathrm{T} / \mathrm{K})$; temp range $200-274 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.1706-1601.52 /(7.059+\mathrm{T} / \mathrm{K})$; temp range $126-192 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.05416-970.771 /(-27.089+\mathrm{T} / \mathrm{K})$; temp range $267-345 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.77294-1482 / 801 /(48.073+\mathrm{T} / \mathrm{K})$; temp range $342-411 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.27411-1097.171 /(-9.657+\mathrm{T} / \mathrm{K})$; temp range $267-411 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)

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\(\log (\mathrm{P} / \mathrm{mmHg})=27.3116-1.9235 \times 10^{3} /(\mathrm{T} / \mathrm{K})-70.2064 \cdot \log (\mathrm{~T} / \mathrm{K})+7.4852 \times 10^{-12} \cdot(\mathrm{~T} / \mathrm{K})+3.6481 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;\) temp range \(88-420 \mathrm{~K}\) (vapor pressure eq., Yaws 1994)
\(596140 \quad\left(50.12^{\circ} \mathrm{C}\right.\), vapor-liquid equilibrium VLE data, Pasanen et al., 2004)
```

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 25610 | (calculated-P/C, Mackay \& Shiu 1981) |
| :--- | :--- |
| 25370 | (calculated-1/ $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975) |
| 26560,15280 | (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 29800 | (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988) |
| 24800 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.40; 2.17, 2.26, 2.43 (quoted; calculated-f const., Rekker 1977)
$1.59,1.32$ (quoted, calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}=1.03 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $30^{\circ} \mathrm{C}$ (flow system, Bufalini \& Altshuller 1965)
$\mathrm{k}_{\mathrm{OH}}=4.08 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (discharge flow system-MS, Morris \& Niki 1971)
$\mathrm{k}_{\mathrm{O} 3}=1.23 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp (Japar et al. 1974)
$\mathrm{k}_{\mathrm{O} 3}=1.03 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp (Huie \& Herron 1975)
$\mathrm{k}_{\mathrm{OH}}=(2.94,2.96) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)
$\mathrm{k}_{\mathrm{O} 3}=1.26 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (static system-chemiluminescence, Adeniji et al. 1981)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=4.20 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom (Singleton \& Cvetanovic 1976; Atkinson \& Pitts Jr. 1977; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}} *=3.53 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297.2 K , measured range $297-425 \mathrm{~K}$ (flash photolysis-resonance fluorescence, Atkinson \& Pitts, Jr. 1977)
$\mathrm{k}_{\mathrm{OH}}=3.13 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{NO} 3}=1.10 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3} \cdot$ molecule $^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.23 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with an estimated lifetime of 5.5 h during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}} *=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3} *=1.35 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3} *=9.64 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=4.15 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: atmospheric lifetime was estimated to be 5.5 h , based on the reaction rate constant $\mathrm{k}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with OH radicals during summer daylight in the gas phase (Altshuller 1991).

Surface water: $\mathrm{t}_{1 / 2}=320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for reaction with OH and $\mathrm{RO}_{2}$ radicals of olefins in aquatic system, and $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$, based on oxidation reaction rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with singlet $\mathrm{O}_{2}$ for unsubstituted olefins in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.2.1
Reported vapor pressures of 1-butene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})$

| Lamb \& Roper 1940 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static method-manometer |  | summary of literature data |  | selected values |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -56.75 | 8549 | -104.8 | 133.3 | -81.5 | 1333 | -8.35 | 93326 |
| -25.3 | 45423 | -89.4 | 666.6 | -72.89 | 2666 | -7.64 | 95992 |
| -22.91 | 50436 | -81.6 | 1333 | -67.41 | 4000 | -6.94 | 98659 |
| -10.60 | 85513 | -73.0 | 2666 | -63.29 | 5333 | -6.26 | 101325 |
| -7.47 | 96992 | -63.4 | 5333 | -59.96 | 6666 | 25.0 | 297309 |
| -0.67 | 125549 | -57.2 | 7999 | -57.15 | 7999 |  |  |
| 0.0 | 128536 | -48.9 | 13332 | -52.52 | 10666 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | -36.2 | 26664 | -48.77 | 13332 | A | 6.84290 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | -6.30 | -21.7 | 53329 | -41.56 | 19998 | B | 926.10 |
| eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | -6.3 | 101325 | -36.10 | 26664 | C | 240.00 |
| A | 6.33816 |  |  | -31.65 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | -6.26 |
| B | 1330.977 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -130 | -27.87 | 39997 |  |  |
| C | 0.0017607 |  |  | -21.62 | 53329 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ |  |
|  |  |  |  | -16.52 | 66661 | at $25^{\circ} \mathrm{C}$ | 20.13 |
|  |  |  |  | -12.16 | 79993 | at bp | 21.92 |



FIGURE 2.1.2.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 1-butene.

### 2.1.2.1.3 2-Methyl-1-butene



Common Name: 2-Methyl-1-butene Synonym:
Chemical Name: 2-methyl-1-butene
CAS Registry No: 563-46-2
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{10}, \mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{C}\left(\mathrm{CH}_{3}\right)=\mathrm{CH}_{2}$
Molecular Weight: 70.133
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-137.53 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
31.2 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6504,0.6451 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, at saturation pressure, Dreisbach 1959; Dean 1985)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 107.8, $108.7 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
7.91 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
58.34, 48.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
215* ( $20^{\circ} \mathrm{C}$, shake flask-GC, measured range $20-60^{\circ} \mathrm{C}$, Pavlova et al. 1966)
155 (estimated-nomograph of Kabadi \& Danner 1979; Brookman et al. 1985)
130 (misquoted from 3-methyl-1-butene, Wakita et al. 1986)
168 (calculated-fragment solubility constants, Wakita et al. 1986)
260 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
137 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
128, 198 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
135540* (interpolated-Antoine eq. regression, temp range -89.1 to $20.2^{\circ} \mathrm{C}$, Stull 1947)
$70242^{*} \quad\left(20.996^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $1.155-62.675^{\circ} \mathrm{C}$, Scott et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87314-1053.780 /\left(232.768+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range 1.155 to $62.675^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Scott et al. 1949)
81320 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87314-1053.8 /\left(233.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -38 to $75^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
$81327^{*}, 81330$ (derived from compiled data, interpolated-Antoine eq., temp range -53.4 to $52.24^{\circ} \mathrm{C}$ Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87314-1053.780 /\left(232.788+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -53.4 to $52.24^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 6474.6 /(\mathrm{T} / \mathrm{K})]+7.751419$; temp range -89.1 to $20.2^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
82830 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.98834-1046.771 /\left(232.181+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ temp range $1.115-63.68^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
99500 (interpolated-Antoine eq., temp range -53 to $52^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84637-1039.69 /\left(236.65+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -53 to $52^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
81360 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99292-1050.937 /(-40.727+\mathrm{T} / \mathrm{K})$; temp range $240-336 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=30.2418-2.2723 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.1482 \cdot \log (\mathrm{~T} / \mathrm{K})+5.2331 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.6802 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $136-465 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
$43080 \quad$ (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.07 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
1.89 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=9.01 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (discharge flow system-MS, Morris \& Niki 1971)
$\mathrm{k}_{\mathrm{OH}}=(6.37 \pm 0.16) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1984)
$\mathrm{k}_{\mathrm{OH}}=9.01 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ to $6.07 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (review, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=(60.7-90.1) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (review, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=6.10 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with an estimated atmospheric lifetime of 2.3 h during summer daylight hours (Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=6.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3}=16.0 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric lifetime $\tau \sim 2.3 \mathrm{~h}$, based on the photooxidation rate constant $\mathrm{k}=6.10 \times 10^{-11} \mathrm{~cm}^{3} \mathrm{molecule}^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical in air during summer daylight (Altshuller 1991).
Surface water: $\mathrm{t}_{1 / 2}=320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for reaction with OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $t_{1 / 2}=7.3 \mathrm{~d}$, based on oxidation reaction rate constant of $3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with singlet oxygen for unsubstituted olefins in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.3.1
Reported aqueous solubilities of 2-methyl-1-butene at various temperatures
Pavlova et al. 1966

| Shake flask-GC |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{\mathbf{3}}$ |
| 20 | 215 |
| 40 | 326 |
| 50 | 250 |
| 60 | 267 |



FIGURE 2.1.2.1.3.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for 2-methyl-1-butene.

TABLE 2.1.2.1.3.2
Reported vapor pressures of 2-methyl-1-butene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t}^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |

Stull $1947 \quad$ Scott et al. $1949 \quad$ Zwolinski \& Wilhoit 1971

| summary of literature data |  | ebulliometry |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -89.1 | 133.3 | 1.155 | 31163 | -53.4 | 1333 | eq. 2 | P/mmHg |
| -72.8 | 666.6 | 6.054 | 38547 | -43.7 | 2666 | A | 6.87314 |
| -64.3 | 1333 | 10.993 | 47357 | -37.5 | 4000 | B | 1053.780 |
| -54.8 | 2666 | 15.973 | 57800 | -32.87 | 5333 | C | 232.788 |
| -44.1 | 5333 | 20.996 | 70242 | -29.13 | 6666 | bp/ $/{ }^{\circ} \mathrm{C}$ | 31.163 |
| -37.3 | 7999 | 26.062 | 84534 | -25.96 | 7999 | $\Delta \mathrm{H}_{\mathrm{V}} / \mathrm{kJ}$ |  |
| -28.0 | 13332 | 31.162 | 101319 | -20.76 | 10666 | at $25^{\circ} \mathrm{C}$ | 25.86 |
| -13.8 | 26664 | 36.308 | 120792 | -16.54 | 13332 | at bp | 25.50 |
| 2.5 | 53329 | 41.500 | 143281 | -8.44 | 19998 |  |  |
| 20.2 | 101325 | 46.728 | 169952 | -2.308 | 26664 |  |  |
|  |  | 52.005 | 198556 | 2.683 | 33331 |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -135 | 57.320 | 232100 | 6.924 | 39997 |  |  |
|  |  | 62.675 | 270083 | 13.936 | 53329 |  |  |
|  |  |  |  | 19.865 | 66661 |  |  |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 31.16 | 24.546 | 79993 |  |  |
|  |  | Antoine eq. |  | 28.623 | 93326 |  |  |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 29.620 | 95992 |  |  |
|  |  | A | 6.87314 | 30.400 | 98659 |  |  |
|  |  | B | 1052.780 | 31.163 | 101325 |  |  |
|  |  | C | 232.788 | 25.0 | 81327 |  |  |



FIGURE 2.1.2.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1-butene.

### 2.1.2.1.4 3-Methyl-1-butene



Common Name: 3-Methyl-1-butene
Synonym:
Chemical Name: 3-methyl-1-butene
CAS Registry No: 563-45-1
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{10},\left(\mathrm{CH}_{3}\right)_{2} \mathrm{CCHCH}=\mathrm{CH}_{2}$
Molecular Weight: 70.133
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -168.43 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
20.1 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6272,0.6219 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, at saturation pressure, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $111.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Ruelle \& Kesselring 1997) 111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
5.36 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
51.19, 41.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ : 130 (shake flask-GC, McAuliffe 1966)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$101325\left(20.2^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -89.1 to $20.2^{\circ} \mathrm{C}$, Stull 1947)
120790* $\quad\left(25.128^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $0.218-51.139^{\circ} \mathrm{C}$, Scott \& Waddington 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82618-1013.474 /\left(236.816+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0.219-51.139^{\circ} \mathrm{C}$ (Antoine eq., ebulliometric method, Scott \& Waddington 1950)
120260 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82618-1013.474 /\left(237.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -47 to $60^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
120000 (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
120270* (derived from compiled data, temp range -62.9 to $40.84^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82618-1013.474 /\left(236.816+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -62.9 to $40.84^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
120180 (interpolated-Antoine eq., temp range -63 to $41^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.82455-1012.37 /\left(236.65+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -63 to $41^{\circ} \mathrm{C}($ Antoine eq., Dean 1985,1992$)$
120300 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.94656-1010.866 /(-36.694+\mathrm{T} / \mathrm{K})$; temp range $237-324 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=31.1486-2.1764 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.6146 \cdot \log (\mathrm{~T} / \mathrm{K})+5.9672 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+4.7555 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $105-450 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 54230 | (calculated-1/K $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975) |
| :--- | :--- |
| 63715,22610 | (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 54700 | (calculated-P/C, Mackay \& Shiu 1981) |
| 43080 | (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988) |

(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
2.07 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
2.05 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=(3.10 \pm 0.31) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299.2 K , measured range $299-433 \mathrm{~K}$ (flash photolysisresonance fluorescence, Atkinson et al. 1977)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=4.30 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom (Singleton \& Cvetanovic 1976; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=3.18 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=9.01 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $6.07 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=3.18 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{NO} 3}=9.8 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=3.18 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=11.0 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=4.15 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2}=320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for reaction with OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $t_{1 / 2}=7.3 \mathrm{~d}$, based on oxidation reaction rate constant $k=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with singlet oxygen for (unsubstituted olefins in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.4.1
Reported vapor pressures of 3-methyl-1-butene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(1a)
$\log P=A-B /(C+T / K)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
Scott \& Waddington $1950 \quad$ Zwolinski \& Wilhoit 1971

| ebulliometry |  |  |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 0.210 | 47363 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 20.06 | -62.9 | 1333 | 17.757 | 93326 |
| 5.112 | 57799 | Antoine eq. |  | -53.4 | 2666 | 18.541 | 95992 |
| 10.053 | 70109 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | -47.3 | 4000 | 19.309 | 98659 |
| 15.033 | 84158 | A | 6.82618 | -42.6 | 5333 | 20.061 | 101325 |
| 20.061 | 101325 | B | 1913.474 | -39.2 | 6666 | 25.0 | 120270 |
| 25.128 | 120790 | C | 236.816 | -36.05 | 7999 |  |  |
| 30.245 | 143268 |  |  | -30.96 | 10666 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 35.402 | 169066 |  |  | -26.82 | 13332 | A | 6.82618 |
| 40.602 | 198543 |  |  | -18.87 | 19998 | B | 1013.474 |
| 45.847 | 232073 |  |  | -12.85 | 26664 | C | 236.816 |
| 51.139 | 280097 |  |  | -7.95 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | 20.061 |
|  |  |  |  | -3.783 | 39997 | $\Delta \mathrm{H}_{\mathrm{V}} / \mathrm{kJ}$ |  |
|  |  |  |  | 3.109 | 53329 | at $25^{\circ} \mathrm{C}$ | 23.85 |
|  |  |  |  | 8.743 | 66661 | at bp | 24.06 |
|  |  |  |  | 13.546 | 79993 |  |  |



FIGURE 2.1.2.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for 3-methyl-1-butene.

### 2.1.2.1.5 2-Methyl-2-butene



Common Name: 2-Methyl-2-butene Synonym:
Chemical Name: 2-methyl-2-butene
CAS Registry No: 513-35-9
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{10}, \mathrm{CH}_{3} \mathrm{CH}=\mathrm{C}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{3}$
Molecular Weight: 70.133
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-133.72 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 38.56 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6623,0.6570 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 105.9, $106.8\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $7.60 \quad$ (Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
54.47, 59.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$215^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $20-60^{\circ} \mathrm{C}$, Pavlova et al. 1966)
325* (calculated-liquid-liquid equilibrium LLE data, temp range 288-333.2 K, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
47876* $\quad\left(18.07^{\circ} \mathrm{C}\right.$, static method, measured range -78.85 to $18.07^{\circ} \mathrm{C}$, Lamb \& Roper 1940)
$\log (\mathrm{P} / \mathrm{mmHg})=9.86840-1773.506 /(\mathrm{T} / \mathrm{K})+0.0035747 \cdot \log (\mathrm{~T} / \mathrm{K}) ;$ temp range -78.85 to $18.07^{\circ} \mathrm{C}$ (static method, Lamb \& Roper 1940)
53329* (21.6, summary of literature data, temp range -75.4 to $38.5^{\circ} \mathrm{C}$, Stull 1947)
57798* (ebulliometry, measured range 3.042 to $70.59^{\circ} \mathrm{C}$, Scott et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91562-1095.088 /\left(232.842+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range 3.042 to $70.59^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Scott et al. 1949)
62140 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91562-1095.088 /\left(233.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -31 to $85^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
62142*, 62140 (derived from compiled data, interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91562-1095.088 /\left(232.842+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -47.7 to $60.0^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
62890, 62140 (calculated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.15017-1146.28 /\left(238.416+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -78.85 to $18.07^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.04808-1099.054 /\left(233.314+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $3.04-70.59^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
62240 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.96659-1124.33 /\left(236.63+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -48 to $60^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
62170 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.04475-1097.501 /(-39.985+\mathrm{T} / \mathrm{K})$; temp range $271-343 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=33.7539-2.426 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.4429 \cdot \log (\mathrm{~T} / \mathrm{K})+9.8488 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+4.7156 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $139-471 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
24650 (calculated-P/C from selected data)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k ; for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}=7.47 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $30^{\circ} \mathrm{C}$ (flow system, Bufalini \& Altshuller 1965)
$\mathrm{k}_{\mathrm{OH}}=11.9 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (discharge flow system-MS, Morris \& Niki 1971)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=5.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ (Herron \& Huie 1973; Furuyama et al. 1974;
Atkinson \& Pitts Jr. 1978; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{O} 3}=4.93 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299 K (Japar et al. 1974)
$\mathrm{k}_{\mathrm{OH}}=4.8 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with atmospheric $\mathrm{t}_{1 / 2}<0.24 \mathrm{~h}$ (Darnall et al.1976, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=8.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1979; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=8.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=54 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (LFE correlation, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=(87.1 \pm 2.6) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1984)
$\mathrm{k}_{\mathrm{NO} 3}=(5.5 \pm 1.2) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} 295 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{O} 3}=4.2 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes $\tau=55 \mathrm{~min}$ and 17 min in clean and moderately polluted atmosphere respectively, $\mathrm{k}_{\mathrm{OH}}=8.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes $\tau=3.2 \mathrm{~h}$ and 1.6 h in clean and moderately polluted atmosphere, respectively; $\mathrm{k}_{\mathrm{NO} 3}=5.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ with calculated lifetimes $\tau=13 \mathrm{~min}$ and 1.3 min in clean and moderately polluted atmosphere, respectively (Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}<0.5 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=4.5 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=8.6 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{NO} 3}=5.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$
$\mathrm{s}^{-1}$; and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=47.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}=8.68 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{O} 3}=(6.79-7.97) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, 296-299 \mathrm{~K}$ (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{O} 3}=4.2 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $25 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=8.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss
rate of $8 \mathrm{~d}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=9.9 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $205 \mathrm{~d}^{-1}$ (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=7.7 \times 10^{-11}$ to $1.19 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ between $297.7-299.5 \mathrm{~K}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{O} 3}=4.2 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $25 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=8.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a
loss rate of $3.8 \mathrm{~d}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=9.9 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $205 \mathrm{~d}^{-1}$ at room temp (Atkinson 1985)
$\mathrm{k}_{\mathrm{NO} 3}=(9.33 \pm 1.18) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} 296 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson 1988)
$\mathrm{k}_{\mathrm{OH}}=8.69 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=6.89 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=4.23 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 198 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=8.69 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=9.33 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 19 90)
$\mathrm{k}_{\mathrm{NO} 3}=9.37 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=8.69 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=9.37 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3} *=4.03 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=5.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right.$ ) atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $\mathrm{t}_{1 / 2}<0.24 \mathrm{~h}$, based on the photooxidation rate constant $\mathrm{k}=4.8 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976);
atmospheric lifetimes, $\tau($ calc $)=0.95 \mathrm{~h}$ for the reaction with $\mathrm{O}_{3}, \tau=3.2 \mathrm{~h}$ with OH radical and $\tau=0.12 \mathrm{~h}$ with $\mathrm{NO}_{3}$ radical, based on the rate constants and environmental concentrations of $\mathrm{OH}, \mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ in the gas phase (Atkinson \& Carter 1984);
calculated lifetimes: $\tau=55 \mathrm{~min}$ due to reaction with $\mathrm{O}_{3}$ in $24-\mathrm{h}$ period, $\tau=3.2 \mathrm{~h}$ with OH radical during daytime, and $\tau=13 \mathrm{~min}$ for $\mathrm{NO}_{3}$ radical during nighttime for "clean" atmosphere; $\tau=17 \mathrm{~min}$ for reaction with $\mathrm{O}_{3}$ in 24 -h period, $\tau=1.6 \mathrm{~h}$ with OH radical during daytime, and $\tau=1.3$ min with $\mathrm{NO}_{3}$ radical during nighttime in "moderately" polluted atmosphere (Atkinson et al. 1984a);
atmospheric lifetimes $\tau($ calc $)=6.38 \mathrm{~h}$ for the reaction with OH radical, $\tau$ (calc) $=0.92 \mathrm{~h}$ with $\mathrm{O}_{3}$ and $\tau$ (calc) $=0.12 \mathrm{~h}$ with $\mathrm{NO}_{3}$ radical in the gas phase (Atkinson 1985).
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for reaction with OH and $\mathrm{RO}_{2}$ radicals respectively in aquatic system, and $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$, based on rate constant of $10^{6} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.5.1
Reported aqueous solubilities of 2-methyl-2-butene at various temperatures

| Pavlova et al. $\mathbf{1 9 6 6}$ |  |  | Góral et al. $\mathbf{2 0 0 4}$ |  |
| :--- | :---: | :---: | :---: | :---: |
|  | shake flask-GC |  | calc-recommended LLE data |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 20 | 215 |  | 15 | 343 |
| 40 | 236 |  | 20 | 334 |
| 50 | 250 |  | 25 | 325 |
| 60 | 267 |  | 40 | 325 |
|  |  |  | 50 | 338 |
|  |  |  | 60 | 361 |



FIGURE 2.1.2.1.5.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for 2-methyl-2-butene.

TABLE 2.1.2.1.5.2
Reported vapor pressures of 2-methyl-2-butene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})$ | $(5)$ |  |  |


| Lamb \& Roper 1940 |  | Stull 1947 |  | Scott et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Static method-manometer |  | Summary of literature data |  | Ebulliometry |  | Selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -78.85 | 97 | -75.4 | 133.3 | 3.042 | 25007 | -47.7 | 1333 |
| -54.78 | 811 | -57.0 | 666.6 | 8.008 | 31172 | -37.8 | 2666 |
| -37.98 | 2696 | -47.0 | 1333 | 12.987 | 38534 | -31.46 | 4000 |
| -29.84 | 4517 | -37.9 | 2666 | 18.033 | 47364 | -26.75 | 5333 |
| -21.06 | 7537 | -26.7 | 5333 | 23.103 | 57798 | -22.92 | 6666 |
| -12.14 | 11767 | -19.4 | 7999 | 28.220 | 70110 | -19.68 | 7999 |
| -3.98 | 18238 | -9.9 | 13332 | 33.373 | 84522 | -14.37 | 10666 |
| 0.0 | 21918 | 4.0 | 26664 | 38.567 | 101319 | -10.06 | 13332 |
| 0.0 | 22025 | 21.6 | 53329 | 43.806 | 120810 | -1.786 | 19998 |
| 2.44 | 24625 | 38.5 | 101325 | 49.078 | 143268 | 4.486 | 26664 |
| 4.51 | 27024 |  |  | 54.399 | 169079 | 9.559 | 33331 |
| 16.31 | 44783 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -133 | 59.753 | 198543 | 13.883 | 39997 |
| 18.07 | 47876 |  |  | 65.151 | 232087 | 21.029 | 53329 |
|  |  |  |  | 70.590 | 272230 | 26.864 | 66661 |
| bp/ $/{ }^{\circ} \mathrm{C}$ | 38.43 |  |  |  |  | 31.834 | 79993 |
| eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  | 36.187 | 93326 |
| A | 9.68640 |  |  |  |  | 36.998 | 95992 |
| B | 1773.506 |  |  |  |  | 37.791 | 98659 |
| C | 0.0035747 |  |  |  |  | 38.568 | 101325 |

TABLE 2.1.2.1.5.2 (Continued)



FIGURE 2.1.2.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-2-butene.

### 2.1.2.1.6 1-Pentene



Common Name: 1-Pentene
Synonym: amylene, $\alpha$-n-amylene, propylethylene
Chemical Name: 1-pentene
CAS Registry No: 109-67-1
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{10}$
Molecular Weight: 70.133
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-165.12 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
29.96 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.6405,0.63533\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Forziati et al. 1950, Dreisbach 1959)
$0.6353 \quad\left(20^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$109.5\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 25.47, 25.20 ( $25^{\circ}$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$5.998 \quad$ (Riddick et al. 1986)
5.81 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}$ ( $\mathrm{J} / \mathrm{mol} \mathrm{K):}$
$53.82,54.4$ (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ): 148 (shake flask-GC, McAuliffe 1966) 191 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
91420* (interpolated-Antoine eq. regression, temp range -80.4 to $30.1^{\circ} \mathrm{C}$, Stull 1947)
$70834 \quad\left(20^{\circ} \mathrm{C}\right.$, static method, measured range $0-200^{\circ} \mathrm{C}$, Day et al. 1948)
$\log (\mathrm{P} / \mathrm{mmHg})=7.40607-1372.194 /(\mathrm{T} / \mathrm{K})$; temp range $0-30^{\circ} \mathrm{C}$ (static method, Day et al. 1948)
$\log (\mathrm{P} / \mathrm{mmHg})=7.31561-1342.407 /(\mathrm{T} / \mathrm{K})$; temp range $40-95^{\circ} \mathrm{C}$ (static method, Day et al. 1948)
84508* (ebulliometry, measured range -0.159 to $61.64^{\circ} \mathrm{C}$, Scott et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85487-1049.00 /\left(233.994+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -0.159 to $61.64^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Scott et al. 1949)
83750* $\quad\left(24.6^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $12.8-30.7^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.78568-1014.293 /\left(229.783+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.8-30.7^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
86500 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84650-1044.9 /\left(234.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -39 to $73^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

85000* (interpolated-Antoine eq., temp range -63 to $41^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84650-1044.895 /\left(233.516+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -63 to $41^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 6931.2 /(\mathrm{T} / \mathrm{K})]+7.914969$; temp range -80.4 to $30.1^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
85020 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.9716-1045.212 /\left(233.598+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.84-30.7^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)
85200 (interpolated-Antoine eq., temp range -55 to $51^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84424-1044.015 /\left(233.50+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -55 to $51^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$
85100 (literature average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.96914-1044.01 /\left(233.49+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
85040 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.96999-1043.962 /(-39.767+\mathrm{T} / \mathrm{K})$; temp range $218-311 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=36.2741-2.4452 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.405 \cdot \log (\mathrm{~T} / \mathrm{K})-7.4629 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+5.4070 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $110-465 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
40330 (calculated-P/C, Mackay \& Shiu 1975; selected, Mills et al. 1982)
41140 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
37520, 22610 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
40300 (calculated-P/C, Mackay \& Shiu 1981)
37520 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
40405 (calculated-P/C, Eastcott et al. 1988)
40280 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
2.20 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
2.69 (calculated-f const., Yalkowsky \& Morozowich 1980)
2.20 (calculated-MCI $\chi$, Murray et al. 1975)
2.80 (selected, Müller \& Klein 1992)
2.3970 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.0* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC determined $\gamma^{\circ}$ in octanol, measured range $20.29-50.2^{\circ} \mathrm{C}$, Gruber et al. 1997)
1.93 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=4.25 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (discharge flow system-MS, Morris \& Niki 1971)
$\mathrm{k}_{\mathrm{O} 3}=1.07 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Japar et al. 1974)
$\mathrm{k}_{\mathrm{O} 3}=5.3 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, 7.4 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $1.07 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (review, Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=3.13 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=1.10 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{O} 3}=1.00 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1994)
$\mathrm{k}_{\mathrm{OH}}=3.14 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}^{*}=10.0 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=4.65 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:

Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for olefins in aquatic system by oxidation with OH and $\mathrm{RO}_{2}$ radicals; while $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$ based on rate constant $\mathrm{k}=3 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.6.1
Reported vapor pressures of 1-pentene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |


| Stull 1947 |  | Scott et al. 1949 |  | Forziati et al. 1950 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -80.4 | 133.3 | -0.159 | 31168 | 12.834 | 53703 | -54.8 | 1333 |
| -63.3 | 666.6 | 4.751 | 38545 | 18.468 | 66797 | -45.1 | 2666 |
| -54.5 | 1333 | 9.706 | 47348 | 24.584 | 63754 | -38.91 | 4000 |
| -46.0 | 2666 | 14.706 | 57789 | 28.900 | 97645 | -34.28 | 5333 |
| -34.1 | 5333 | 19.750 | 70094 | 29.362 | 99227 | -30.53 | 6666 |
| -27.1 | 7999 | 24.834 | 84508 | 29.796 | 100727 | -27.36 | 7999 |
| -17.7 | 13332 | 29.967 | 101322 | 30.289 | 102453 | -22.14 | 10666 |
| -3.40 | 26664 | 35.142 | 120813 | 30.723 | 103988 | -17.92 | 13332 |
| 12.8 | 53329 | 40.359 | 143295 |  |  | -9.789 | 19998 |
| 30.1 | 101325 | 45.614 | 169079 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 29.968 | -3.640 | 26664 |
|  |  | 50.914 | 198557 |  |  | 1.368 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | 56.253 | 232061 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 5.624 | 39997 |
|  |  | 61.641 | 270071 | A | 6.78568 | 12.664 | 53329 |
|  |  |  |  | B | 1014.294 | 18.416 | 66661 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 29.97 | C | 229.783 | 23.319 | 79993 |
|  |  | Antoine eq. |  |  |  | 27.616 | 93326 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | 28.417 | 95992 |
|  |  | A | 6.85487 |  |  | 29.201 | 98659 |
|  |  | B | 1049.00 |  |  | 29.968 | 101325 |
|  |  | C | 233.994 |  |  | 25.0 | 85020 |
|  |  |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 6.84650 |
|  |  |  |  |  |  | B | 1044.895 |
|  |  |  |  |  |  | C | $233.516$ |
|  |  |  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 29.968 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 25.47 |
|  |  |  |  |  |  | at bp | 25.20 |



FIGURE 2.1.2.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for 1-pentene.

## TABLE 2.1.2.1.6.2

Reported octanol-air partition coefficients of 1-pentene at various temperatures and temperature dependence equations

Gruber et al. 1997

| GC det'd activity coefficient |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\boldsymbol{\operatorname { l o g } K _ { \text { OA } }}$ |
| 20.29 | 1.995 |
| 30.3 | 1.852 |
| 40.4 | 1.740 |
| 50.28 | 1.630 |



FIGURE 2.1.2.1.6.2 Logarithm of $K_{O A}$ versus reciprocal temperature for 1-pentene.

### 2.1.2.1.7 cis-2-Pentene

$\qquad$
Common Name: cis-2-Pentene
Synonym: (Z)-2-pentene
Chemical Name: cis-2-pentene
CAS Registry No: 627-20-3
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{10}$
Molecular Weight: 70.133
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ : -151.36 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 36.93 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6556,0.6504\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 107.0, $107.8\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 7.112 (Riddick et al. 1986)
7.11 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
58.39, 52.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
203 (shake flask-GC, cis-trans form not specified, McAuliffe 1966)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
57795* $\quad\left(21.541^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $1.595-68.842^{\circ} \mathrm{C}$, Scott \& Waddington 1950) $\log (\mathrm{P} / \mathrm{mmHg})=6.87540-1069.460 /\left(240.786+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $1.595-68.842^{\circ} \mathrm{C}$ (Antoine eq., ebulliometric method, Scott \& Waddington 1950)
65940 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87274-1068.0 /\left(231.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -33 to $82^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

66000, 65941 (interpolated-Antoine eq., derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87274-1067.951 /\left(230.585+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -48.7 to $58.31^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
65950 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.99984-1069.227 /\left(230.757+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $1.595-68.88^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
66640 (interpolated-Antoine eq., Dean 1985, 1992)
66000 (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.96798-1052.44 /\left(228.693+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) $\log (\mathrm{P} / \mathrm{mmHg})=6.84308-1052.44 /\left(228.69+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -49 to $58^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 65970 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99069-1064.178 /(-43.035+\mathrm{T} / \mathrm{K})$; temp range $234-318 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=34.0427-2.4524 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.5014 \cdot \log (\mathrm{~T} / \mathrm{K})-5.0816 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+4.3638 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $122-476 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
22800 (calculated-P/C, Mackay \& Shiu 1981)
22770 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
$2.20 \quad$ (calculated $-\pi$ substituent constant, Hansch et al. 1968)
2.20 (calculated-MCI $\chi$, cis-trans form not specified, Murray et al. 1975)
2.3772 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.80 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom (Herron \& Huie 1973; quoted,
Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=6.20 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1979; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{OH}}=(6.23 \pm 0.1) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1984)
$\mathrm{k}_{\mathrm{OH}}=(65.4-65.9) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298-303 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=6.50 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=6.50 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with an estimated atmospheric lifetime of 2.29 h in summer daylight
(Altshuller 1991)
$\mathrm{k}_{\mathrm{OH}}=6.5 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: photooxidation reaction rate constant $\mathrm{k}=6.50 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical in air (Atkinson 1990, Altshuller 1991) with an estimated atmospheric lifetime of 2.29 h in summer daylight (Altshuller 1991).
Surface water: $t_{1 / 2} \sim 320 \mathrm{~h}$ for oxidation by OH radicals, $\mathrm{t}_{1 / 2}=9 \times 10^{4} \mathrm{~d}$ for olefins in aquatic system, and $t_{1 / 2}=$ 7.3 d based on rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of unsubstituted olefins by singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.7.1
Reported vapor pressures of cis-2-pentene at various temperatures

| Scott \& Waddington $\mathbf{1 9 5 0}$ |  |  |  |
| :---: | ---: | :--- | :---: |
| ebulliometric method |  |  |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 1.595 | 25009 | 58.070 | 198556 |
| 6.522 | 31163 | 63.456 | 232087 |
| 11.486 | 38546 | 68.882 | 270057 |
| 16.494 | 47357 |  |  |
| 21.541 | 57795 | $\operatorname{log~P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| 26.633 | 70102 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 36.94 |
| 31.766 | 84518 |  | $\mathrm{P} / \mathrm{mmHg}$ |
| 36.944 | 101329 | A | 6.87540 |
| 42.161 | 120804 | B | 1069.460 |
| 47.423 | 143281 | C | 240.786 |
| 52.724 | 169066 |  |  |

### 2.1.2.1.8 <br> 2-Methyl-1-pentene



Common Name: 2-Methyl-1-pentene
Synonym:
Chemical Name: 2-methyl-1-pentene
CAS Registry No: 763-29-1
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{12} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{2} \mathrm{C}\left(\mathrm{CH}_{3}\right) \mathrm{CH}_{2}$
Molecular Weight: 84.159
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-135.7 (Dreisbach 1959; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
60.7 (Dreisbach 1959)
62.1 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6799,0.6751 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
123.8, $124.7\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 133.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
78.0 (shake flask-GC, McAuliffe 1966)
98.2 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
27464 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88772-1154.7 /\left(227.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -14 to $100^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
26000, 26051 (interpolated-Antoine eq., derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85030-1138.516 /\left(224.764+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -30.1 to $85.16^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85030-1138.516 /\left(224.70+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -30 to $85^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 ) 26060 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.89056-1091.679 /(-46.306+\mathrm{T} / \mathrm{K})$; temp range $265-333 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99434-1148.616 /(-49.853+\mathrm{T} / \mathrm{K})$; temp range: $275-344 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=32.9509-2.8171 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.9572 \cdot \log (\mathrm{~T} / \mathrm{K})-8.7635 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.1710 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $137-507 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
28100 (calculated-P/C, Mackay \& Shiu 1981)
28093 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=1.05 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ under atmospheric conditions (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=(8.76 \pm 0.14) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1984)
$\mathrm{k}_{\mathrm{OH}}=62.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1985, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=6.3 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=15.0 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$, based on rate constant $\mathrm{k}=1.0 \times 10^{6} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of substituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

### 2.1.2.1.9 4-Methyl-1-pentene



Common Name: 4-Methyl-1-pentene
Synonym:
Chemical Name: 4-methyl-1-pentene
CAS Registry No: 691-37-2
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{12}$
Molecular Weight: 84.159
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-153.6 (Dreisbach 1959; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
$53.88 \quad$ (Dreisbach 1959)
53.9 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6642,0.6594\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1059)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$126.7\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966, Ruelle \& Kesselring 1997)
$127.6 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
133.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
48.0 (shake flask-GC, McAuliffe 1966)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
35600 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87757-1130.0 /\left(229.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -20 to $91^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

36104, 36100 (derived from compiled data, interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83529-1121.302 /\left(229.687+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -37.5 to $76.75^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83529-1121.302 /\left(229.687+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -38 to $77^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992) 36110 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.94694-1114.082 /(-44.332+\mathrm{T} / \mathrm{K})$; temp range $265-333 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=44.7746-2.7364 \times 10^{3} /(\mathrm{T} / \mathrm{K})-14.283 \cdot \log (\mathrm{~T} / \mathrm{K})+7.31 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+4.8402 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $120-496 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
62270 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
65200, 34220 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
63200 (calculated-P/C, Mackay \& Shiu 1981)
63270 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {Ow }}$ :
$2.50 \quad$ (calculated $-\pi$ constant, Hansch et al. 1968)
2.51 (calculated-MCI $\chi$, Murray et al. 1975)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{03}=1.06 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson \& Carter 1984)
$\mathrm{k}_{03}=9.2 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$, based on rate constant $\mathrm{k}=1.0 \times 10^{6} \mathrm{M}-\mathrm{s}^{-1}$ for oxidation of substituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

### 2.1.2.1.10

1-Hexene


Common Name: 1-Hexene
Synonym: $\alpha$-hexene
Chemical Name: 1-hexene
CAS Registry No: 646-04-8
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{12} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{3} \mathrm{CHCH}_{2}$
Molecular Weight: 84.159
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -139.76 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
63.48 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.6732,0.6685 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$125.0\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Wang et al. 1992; Ruelle \& Kesselring 1997)
$125.9 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
133.2 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.347 (Riddick et al. 1986)
9.35 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 70.1, 61.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
50.0 (shake flask-GC, McAuliffe 1966)
65.5 (shake flask-titration, Natarajan \& Venkatachalam 1972)
$65.5,54.12,42.16\left(25,30,35^{\circ} \mathrm{C}\right.$, shake flask-titration, in $0.001 \mathrm{M} \mathrm{HNO}_{3}$ solution, Natarajan \& Venkatachalam 1972)
55.4 (shake flask-GC, Leinonen \& Mackay 1973)
$60.0 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, Budantseva et al. 1976)
69.7 (generate column-GC, Tewari et al. 1982a)

100, $53 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, "best" values, IUPAC Solubility Data Series, Shaw 1989a)
$\ln x=-268.791+11353.70 /(\mathrm{T} / \mathrm{K})+38.4871 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature
calorimetric and solubility data, Tsonopoulos 2001)
$\ln x=-276.423+11833.54 /(\mathrm{T} / \mathrm{K})+39.5126 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from direct fit of
solubility data, Tsonopoulos 2001)
51.43* (calculated-liquid-liquid equilibrium LLE data, temp range 293.2-494.3 K, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
22300* (Antoine eq. regression, temp range -57.5 to $66^{\circ} \mathrm{C}$, Stull 1947)
$23500^{*} \quad\left(23.7^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $15.9-64.3^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86573-1152.971 /\left(225.849+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.9-64.3^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1950)
25000 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86572-1152.971 /\left(226.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -12 to $79^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
24800*, 24798 (interpolated-Antoine eq., derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86573-1152.971 /\left(225.849+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -29.3 to $86.64^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7787.6 /(\mathrm{T} / \mathrm{K})]+7.930324$; temp range -57.5 to $66^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
24800 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.99426-1154.952 /\left(226.002+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.89-64.311^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)
24800 (interpolated-Antoine eq., temp range -16 to $64^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85770-1148.62 /\left(225.25+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -16 to $64^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 24800 (selected lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=5.98260-1148.62 /\left(225.346+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 24800 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.98336-1149.029 /(-47.755+\mathrm{T} / \mathrm{K})$; temp range $273-343 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=33.4486-2.6221 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.1784 \cdot \log (\mathrm{~T} / \mathrm{K})+3.093 \times 10^{-12} .(\mathrm{T} / \mathrm{K})+3.678 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 133-504 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 41750 | (calculated-P/C, Mackay \& Shiu 1975) |
| :--- | :--- |
| 44080 | (calculated-1/K $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975) |
| 51790,34220 | (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975) |
| 41800 | (calculated-P/C, Mackay \& Shiu 1981) |
| 47230 | (calculated- $\chi$, Nirmalakhandan \& Speece 1988) |
| 41640 | (calculated-P/C, Eastcott et al. 1988) |
| 29940 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.39 (generator column-GC, Tewari et al. 1982a,b)
3.47 (calculated-activity coeff. $\gamma$, Wasik et al. 1981)
3.48 (calculated-activity coeff. $\gamma$, Wasik et al. 1982)
3.39, 3.40 (generator column-GC, calculated-activity coeff. $\gamma$, Schantz \& Martire 1987)
3.40 (recommended, Sangster 1989)
3.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.50* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\circ}$ in octanol, measured range $20.29-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997)
2.41 (calculated-measured $\gamma^{\circ}$ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=0.90 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Cadle \& Schadt 1952)
$\mathrm{k}_{\mathrm{O} 3}=1.00 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Hanst et al. 1958)
$\mathrm{k}_{\mathrm{O} 3}=1.10 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $30^{\circ} \mathrm{C}$ (flow system, Bufalini \& Altshuller 1965)
$\mathrm{k}_{\mathrm{O} 3}=1.40 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (static system-chemiluminescence, Cox \& Penkett 1972)
$\mathrm{k}_{\mathrm{O} 3}=1.10 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299 K (static system-chemiluminescence, Stedman et al. 1973)
$\mathrm{k}_{\mathrm{O} 3}=1.11 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (static system-chemiluminescence, Japar et al. 1974)
$\mathrm{k}_{\mathrm{O} 3}=1.08 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (static system-chemiluminescence, Adeniji et al. 1981)
$\mathrm{k}_{\mathrm{O} 3}=1.21 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (static system-chemiluminescence, Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{O} 3}=(0.91$ to 1.36$) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 294-303 K (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=3.68 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)

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\mp@subsup{k}{\textrm{OH}}{}=(3.75-3.25)\times1\mp@subsup{0}{}{-11}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1}\mathrm{ at 295-303 K (Atkinson 1985)}
\mp@subsup{k}{\textrm{OH}}{}=(32.9-37.5)\times1\mp@subsup{0}{}{-12}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1}\mathrm{ at 295-303 K (Atkinson 1989)}
k}\mp@subsup{\textrm{OH}}{\textrm{OH}}{=3.18\times1\mp@subsup{0}{}{-11}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1},\mp@subsup{\textrm{k}}{\textrm{O}3}{}=1.17\times1\mp@subsup{0}{}{-17}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1}\mathrm{ at 298 K (Atkinson 1990)}
\mp@subsup{k}{03}{}}=1.10\times1\mp@subsup{0}{}{-17}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1}\mathrm{ at }298\textrm{K}\mathrm{ (recommended, Atkinson 1997)
\mp@subsup{k}{\textrm{OH}}{}=3.7\times1\mp@subsup{0}{}{-11}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1},\mp@subsup{\textrm{k}}{\textrm{O}3}{*}=11.0\times1\mp@subsup{0}{}{-18}\mp@subsup{\textrm{cm}}{}{3}\mathrm{ molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1}\mathrm{ , and }\mp@subsup{\textrm{k}}{\textrm{O}(3P)}{}=4.65\times1\mp@subsup{0}{}{-12}\mp@subsup{\textrm{cm}}{}{3}
    molecule}\mp@subsup{}{}{-1}\mp@subsup{\textrm{s}}{}{-1}\mathrm{ for reaction with O(3P) atom at 298 K (recommended, Atkinson 1997)
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Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$, based on rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.10.1
Reported aqueous solubilities of 1 -hexene at various temperatures

Góral et al. 2004
Calc-recommended LLE data

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| :---: | :---: |
| 20 | 56.11 |
| 25 | 51.43 |
| 36.8 | 51.43 |
| 93.3 | 102.9 |
| 148.8 | 392.8 |
| 204.4 | 2151 |
| 221.1 | 3740 |



FIGURE 2.1.2.1.10.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-hexene.

TABLE 2.1.2.1.10.2
Reported vapor pressures and octanol-air partition coefficients of 1-hexene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$

Vapor pressure $\quad \log K_{\text {OA }}$

| Stull 1947 |  | Forziati et al. 1950 |  | Zwolinski \& Wilhoit 1971 |  | Gruber et al. 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Summary of literature data |  | Ebulliometry |  | Selected values |  | GC det'd activity coefficient |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} \mathrm{K}_{\text {OA }}$ |
| -57.5 | 133.3 | 15.890 | 16645 | -29.30 | 1333 | 20.29 | 2.503 |
| -38.0 | 666.6 | 19.950 | 19946 | -18.65 | 2666 | 30.3 | 2.331 |
| -28.1 | 1333 | 23.720 | 23485 | -11.88 | 4000 | 40.4 | 2.20 |
| -17.2 | 2666 | 28.762 | 28990 | -6.81 | 5333 | 50.28 | 2.068 |
| -5.0 | 5333 | 33.399 | 34936 | -2.70 | 6666 |  |  |
| 2.8 | 7999 | 38.993 | 43366 | 0.776 | 7999 |  |  |
| 13.0 | 13332 | 44.763 | 53705 | 8.482 | 10666 |  |  |
| 29.0 | 26664 | 50.914 | 66798 | 11.109 | 13332 |  |  |
| 46.8 | 53329 | 62.323 | 97648 | 20.006 | 19998 |  |  |
| 66.0 | 101325 | 62.827 | 99230 | 26.736 | 26664 |  |  |
|  |  | 63.299 | 100730 | 32.215 | 33331 |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | 62.837 | 102457 | 38.871 | 39997 |  |  |
|  |  | 64.311 | 103995 | 44.569 | 53329 |  |  |
|  |  |  |  | 50.859 | 66661 |  |  |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 56.219 | 79993 |  |  |
|  |  | A | 6.86573 | 60.915 | 93326 |  |  |
|  |  | B | 1152.971 | 61.790 | 95992 |  |  |
|  |  | C | 225.849 | 62.647 | 98659 |  |  |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 63.485 | 63.585 | 101325 |  |  |
|  |  |  |  | 25.0 | 24798 |  |  |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  |  |  | A | 6.86572 |  |  |
|  |  |  |  | B | 1152.971 |  |  |
|  |  |  |  | C | 225.849 |  |  |
|  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 63.485 |  |  |
|  |  |  |  | $\begin{array}{r} \Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ} \mathrm{~m} \\ \text { at } 25^{\circ} \mathrm{C} \end{array}$ | 28.28 |  |  |
|  |  |  |  | at bp | 30.63 |  |  |



FIGURE 2.1.2.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexene.


FIGURE 2.1.2.1.10.3 Logarithm of $K_{O A}$ versus reciprocal temperature for 1-hexene.

### 2.1.2.1.11 1-Heptene



Common Name: 1-Heptene
Synonym: 1-heptylene, $\alpha$-heptene
Chemical Name: 1-heptene
CAS Registry No: 592-76-7
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{14}, \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{4} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 98.186
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -118.9 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 93.64 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6970,0.6927 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Forziati et al. 1950; Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $140.9 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987; Ruelle \& Kesselring 1997) $141.8 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density) 155.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 35.65, $31.09\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 12.401 (Riddick et al. 1986) 12.66 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 82.5, 77.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999) Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
31.03, 27.6, $24.06\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}, 30^{\circ} \mathrm{C}\right.$, shake flask-titration, in $0.001 \mathrm{M} \mathrm{HNO}_{3}$ solution, Natarajan \& Venkatachalam 1972)
18.16 (generator column-GC, Tewari et al. 1982a)
23.6 (calculated-activity coeff. $\gamma$ and $\mathrm{K}_{\mathrm{OW}}$, Tewari et al. 1982b)
$19,25,32,38\left(10,20,24,30^{\circ} \mathrm{C}\right.$, "best values", IUPAC Solubility Data Series, Shaw 1989a)
$15.27,13.6,13.1\left(10,20,30^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$7690^{*} \quad\left(25.5^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $21.6-94.5^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90069-1257.505 /\left(219.179+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $21.6-94.5^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1950)
7510 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90069-1257.505 /\left(219.18+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10-128^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
$26663^{*}\left(53.17^{\circ} \mathrm{C}\right.$, temp range $53.17-93.61^{\circ} \mathrm{C}$, Eisen \& Orav 1970 ; quoted, Boublik et al. 1984)
7506*, 7510 (derived from compiled data, interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90069-1257.505 /\left(219.179+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -6.07 to $118.44^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8643.2 /(\mathrm{T} / \mathrm{K})]+7.991519$; temp range -35.8 to $98.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
7520, 7530 (interpolated-Antoine equations., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.04107-1266.473 /\left(220.202+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $21.6-94.53^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.03512-1263.343 /\left(219.922+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $54.17-93.61^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
7515 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91087-1258.345 /\left(219.30+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -6 to $118^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$ 7500 (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.02677-1258.34 /\left(219.299+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 7500 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99079-1237.44 /(-56.26+\mathrm{T} / \mathrm{K})$; temp range $311-368 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=38.1255-3.064 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.679 \cdot \log (\mathrm{~T} / \mathrm{K})+1.2244 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+3.668 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $154-537 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
40580 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.99 (generator column-concn. ratio-GC, Tewari et al. 1982a,b)
4.09 (calculated-activity coeff. $\gamma$, Wasik et al. 1982)
4.06 (generator column-GC, Schantz \& Martire 1987)
3.99 (recommended, Sangster 1989, 1993)
3.99 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=8.1 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Cadle \& Schadt 1952)
$\mathrm{k}_{\mathrm{O} 3}=1.73 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (static system-chemiluminescence, Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=3.97 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=40.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $36.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K and 305 K respectively (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=4.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=1.73 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=4.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=12.0 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$, based on rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.11.1
Reported vapor pressures of 1 -heptene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

Zwolinski \& Wilhoit 1971

| Forziati et al. 1950 |  | Eisen \& Orav 1970 |  | Zwolinski \& Wilhoit 1971 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Ebulliometry |  | in Boublik et al. 1984 |  | Selected values |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 21.609 | 6485 | 53.17 | 26663 | -6.07 | 1333 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 25.492 | 7691 | 65.06 | 39997 | 5.39 | 2666 | A | 6.90069 |
| 28.768 | 8991 | 73.32 | 53329 | 12.68 | 4000 | B | 1257.505 |
| 34.525 | 11700 | 80.07 | 66661 | 18.15 | 5333 | C | 219.179 |
| 38.281 | 13845 | 85.82 | 79993 | 22.569 | 6666 | bp/ ${ }^{\circ} \mathrm{C}$ | 93.643 |
| 42.564 | 16644 | 90.86 | 93325 | 26.306 | 7999 |  |  |
| 46.923 | 19945 | 91.33 | 94659 | 32.443 | 10666 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ m |  |
| 50.970 | 23482 | 91.79 | 95992 | 37.418 | 13332 | at $25^{\circ} \mathrm{C}$ | 31.09 |
| 56.384 | 28988 | 92.25 | 97325 | 46.982 | 19998 | at bp | 35.65 |
| 67.366 | 43366 | 92.71 | 98658 | 54.212 | 26664 |  |  |
| 73.563 | 53705 | 93.16 | 99991 | 60.096 | 33331 |  |  |
| 80.179 | 66801 | 93.61 | 101325 | 65.095 | 39997 |  |  |
| 92.391 | 97650 |  |  | 73.357 | 53329 |  |  |
| 92.941 | 99233 |  |  | 80.104 | 66661 |  |  |
| 93.444 | 100733 |  |  | 84.853 | 79993 |  |  |
| 94.022 | 102462 |  |  | 90.888 | 93326 |  |  |
| 94.531 | 104002 |  |  | 91.826 | 95992 |  |  |
|  |  |  |  | 92.744 | 98659 |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | 93.643 | 101325 |  |  |
| A | 6.90069 |  |  | 25.0 | 7506 |  |  |
| B | 1257.505 |  |  |  |  |  |  |
| C | 219.179 |  |  |  |  |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 93.643 |  |  |  |  |  |  |



FIGURE 2.1.2.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for 1-heptene.

### 2.1.2.1.12

1-Octene


Common Name: 1-Octene
Synonym: $\alpha$-octene, caprylene, $\alpha$-octylene
Chemical Name: 1-octene
CAS Registry No: 111-66-0
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{16} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{5} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 112.213
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-101.7 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
121.29 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7149,0.7109 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$154.9 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
177.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 40.35, $33.95\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 15.569 (Riddick et al. 1986) 15.31 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 89.29,86.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
2.70 (shake flask-GC, McAuliffe 1966)
4.10 (generator column-GC, Tewari et al. 1982a)
6.82 (calculated-activity coeff. $\gamma$ and $\mathrm{K}_{\mathrm{OW}}$, Tewari et al. 1982b)
2.70, 22.2 (quoted, IUPAC Solubility Data Series, Shaw 1989)
2.93, $2.93\left(25,37.78^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
6382* $\quad\left(44.893^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $44.893-122.223^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93262-1353.486 /\left(212.765+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $44.8-122.2^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1950)
2317 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93263-1253.5 /\left(212.764+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-151^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

2320* (interpolated-Antoine eq., temp range $15.38-147.54^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93263-1253.486 /\left(212.764+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15.38-147.54^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
2320 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.06421-1356.472 /\left(213.099+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $44.89-122.2^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data Forziati et al. 1950, Boublik et al. 1984)
2320 (interpolated-Antoine eq., temp range $15-147^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93495-1355.46 /\left(213.05+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $15-147^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
2300 (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.05985-1355.46 /\left(213.054+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
2320 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.05178-1350.245 /(-60.716+\mathrm{T} / \mathrm{K})$; temp range $317-400 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=56.1183-3.7657 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.006 \cdot \log (\mathrm{~T} / \mathrm{K})+7.7387 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-1.3036 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $171-567 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
91700 (calculated-P/C, Mackay \& Shiu 1975; selected, Mills et al. 1982)
96440 (calculated-1/ $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
101000, 75000 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
96400 (calculated-P/C, Mackay et al. 1981; Eastcott et al. 1988)
74860 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
63500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.57 (generator column-GC, Tewari et al. 1982a)
4.76 (calculated-activity coeff. $\gamma$, Wasik et al. 1981, 1982)
4.56, 4.72 (generator column-GC, calculated-activity coeff. $\gamma$, Schantz \& Martire 1987)
4.57 (recommended, Sangster 1989)
4.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
3.53 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k ; for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=8.1 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in air (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=4.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{O} 3}=1.70 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.10 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom in gas phase (Paulson \& Seinfeld 1992)
$\mathrm{k}_{\mathrm{O} 3}=14.0 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$, based on rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.12.1
Reported vapor pressures of 1 -octene at various temperatures and the coefficients for the vapor pressure equations
$\log P=A-B /(T / K)$
$\log P=A-B /\left(C+t /{ }^{\circ} C\right)$
$\log P=A-B /(C+T / K)$
$\log P=A-B /(T / K)-C \cdot \log (T / K)$

Forziati et al. 1950

| ebulliometry |  |  |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 44.893 | 6382 | 121.075 | 100743 | 15.38 | 1333 | 118.362 | 93326 |
| 48.975 | 7690 | 121.685 | 102474 | 27.57 | 2666 | 119.355 | 95992 |
| 52.140 | 8994 | 122.223 | 102019 | 35.33 | 4000 | 120.328 | 98659 |
| 55.581 | 10330 |  |  | 41.15 | 5333 | 121.2880 | 101325 |
| 58.557 | 11720 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 45.848 | 6666 | 25.0 | 2320 |
| 62.557 | 13844 | A | 6.93262 | 49.820 | 7999 |  |  |
| 67.096 | 16644 | B | 1353.486 | 56.343 | 10666 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 71.736 | 19945 | C | 212.764 | 61.630 | 13332 | A | 6.93263 |
| 76.022 | 23482 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 121.280 | 71.789 | 19998 | B | 1353.486 |
| 81.779 | 2890 |  |  | 79.645 | 26664 | C | 212.764 |
| 87.053 | 34934 |  |  | 85.710 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | 121.280 |
| 93.428 | 43366 |  |  | 91.014 | 39997 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ} \mathrm{mo}$ |  |
| 106.997 | 66806 |  |  | 99.778 | 53329 | at $25^{\circ} \mathrm{C}$ | 37.95 |
| 119.967 | 97658 |  |  | 106.932 | 66661 | at bp | 33.76 |
| 120.539 | 99242 |  |  | 113.026 | 79993 |  |  |



FIGURE 2.1.2.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-octene.

### 2.1.2.1.13 <br> 1-Nonene



Common Name: 1-Nonene
Synonym: $\alpha$-nonene, $n$-heptylethylene, 1-nonylene
Chemical Name: 1-nonene
CAS Registry No: 124-11-8
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{18} ; \mathrm{CH}_{3}\left(\mathrm{CH}_{2}\right)_{6} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 126.239
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-81.3 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 146.9 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7292,0.7235\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 173.1, $174.1\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 199.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 45.52, $36.31\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 19.075 (Riddick et al. 1986) 19.37 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 104.23, 96.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.63 (estimated-nomograph, Brookman et al. 1986)
1.12 (generator column-GC, Tewari et al. 1982a)
2.09 (calculated-activity coeff. $\gamma$ and $\mathrm{K}_{\mathrm{ow}}$, Tewari et al. 1982b)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$6385^{*} \quad\left(66.607^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $66.607-147.860^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95389-1435.359 /\left(205.535+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $66.6-147.9^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1950)
712 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95387-1435.295 /\left(205.535+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25-173^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
707*, 712 (derived from compiled data, extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95430-1436.20 /\left(205.69+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35-175^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
710 (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.07920-1436.20 /\left(205.690+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
712 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.07341-1432,435 /(-67.884+\mathrm{T} / \mathrm{K})$; temp range $339-423 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=60.6089-4.2023 \times 10^{3} /(\mathrm{T} / \mathrm{K})-19.446 \cdot \log (\mathrm{~T} / \mathrm{K})+7.8308 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.591 \times 10^{-13} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 192-593 K (vapor pressure eq., Yaws 1994)
$650.4 \quad\left(23.25^{\circ} \mathrm{C}\right.$, transpiration method, Verevkin et al. 2000)
$\ln (\mathrm{P} / \mathrm{Pa})=24.60-5379 /(\mathrm{T} / \mathrm{K})$; temp range $278.5-318.3 \mathrm{~K}$ (transpiration method, Verevkin et al. 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
80450 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
5.15 (generator column-GC, Tewari et al. 1982a,b)
5.34 (calculated-activity coeff. $\gamma$, Wasik et al. 1981, 1982)
5.31 (calculated-activity coeff. $\gamma$, Schantz \& Martire 1987)
5.15 (recommended, Sangster 1989)
5.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
3.83 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$, based on rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.13.1
Reported vapor pressures of 1 -nonene at various temperatures and the coefficients for the vapor pressure equations
$\log P=A-B /(T / K)$
$\log P=A-B /\left(C+t /{ }^{\circ} C\right)$
$\log P=A-B /(C+T / K)$
$\log P=A-B /(T / K)-C \cdot \log (T / K)$

Forziati et al. 1950

| ebulliometry |  |  |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 66.607 | 6385 | 146.091 | 99242 | 35.55 | 1333 | 143.805 | 93326 |
| 70.874 | 7691 | 146.653 | 100742 | 48.38 | 2666 | 144.848 | 95992 |
| 74.517 | 8994 | 147.289 | 102474 | 56.55 | 4000 | 145.869 | 98659 |
| 77.861 | 10331 | 147.860 | 104020 | 62.67 | 5333 | 146.868 | 101325 |
| 81.001 | 11722 |  |  | 67.612 | 6666 | 25.0 | 706.6 |
| 85.202 | 13805 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 146.868 | 71.790 | 7999 |  |  |
| 89.942 | 16644 |  |  | 78.651 | 10666 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 94.829 | 19945 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 84.210 | 13332 | A | 6.95387 |
| 99.341 | 23482 | A | 6.95389 | 94.889 | 19998 | B | 1435.359 |
| 110.935 | 34934 | B | 1435.359 | 102.956 | 26664 | C | 205.535 |
| 117.622 | 43364 | C | 146.868 | 109.518 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | 146.868 |
| 124.521 | 53707 |  |  | 115.090 | 39997 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ} \mathrm{m}$ |  |
| 131.881 | 66806 |  |  | 124.295 | 53329 | at $25^{\circ} \mathrm{C}$ | 36.32 |
| 139.859 | 83770 |  |  | 131.808 | 66661 | at bp | 45.52 |
| 145.488 | 97658 |  |  | 138.204 | 79993 |  |  |



FIGURE 2.1.2.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for 1-nonene.

### 2.1.2.1.14 <br> 1-Decene



Common Name: 1-Decene
Synonym: $\alpha$-decene
Chemical Name: 1-decene
CAS Registry No: 872-05-9
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{20}$
Molecular Weight: 140.266
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-66.3 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 170.5 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.7408,0.7369\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Forziati et al. 1950; Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$189.3\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987; Ruelle \& Kesselring 1997)
$190.3 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
222.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 50.43, 38.66 ( $25^{\circ}$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 21.75 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 106.8, 105.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
5.70 (shake flask-titration with bromine, Natarajan \& Venkatachalam 1972; quoted Shaw 1989)
11.0, $8.50,5.70\left(15,20,25^{\circ} \mathrm{C}\right.$, shake flask-titration, in $0.001 \mathrm{M} \mathrm{HNO}_{3}$ solution, Natarajan \& Venkatachalam 1972)
0.161 (calculated- $\mathrm{K}_{\text {OW }}$, Wang et al. 1992)
0.433 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
$0.222,0.344$ (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997) $0.429,4.29,70.13\left(101,151.5,202^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$133.3^{*} \quad\left(14.7^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $14.7-192.0^{\circ} \mathrm{C}$, Stull 1947)
$6397^{*} \quad\left(86.774^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $86.774-171.605^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.96036-1501.812 /\left(197.578+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $86.7-171.6^{\circ} \mathrm{C}$ (Antoine eq., ebulliometrymanometer measurements, Forziati et al. 1950)
218 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.96034-1501.872 /\left(197.58+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25-253^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
218* (extrapolated-Antoine eq., temp range $54.4-199.3^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.96034-1501.872 /\left(197.578+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $54.4-199.3^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{kPa})=6.07985-1497.943 /\left(197.102+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $86.77-171.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)
215 (extrapolated-Antoine eq., temp range: $54-199^{\circ} \mathrm{C}$, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93477-1484.98 /\left(195.707+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range: $54-199^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$
210 (quoted lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.05967-1484.98 /\left(195.707+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) 223 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.12458-1528.811 /(-72.566+\mathrm{T} / \mathrm{K})$; temp range $383-445 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=2.2678-3.1244 \times 10^{3} /(\mathrm{T} / \mathrm{K})+5.432 \cdot \log (\mathrm{~T} / \mathrm{K})-2.0137 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.1221 \times 10^{-5} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 207-617 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, log $\mathrm{K}_{\mathrm{Ow}}$ :
4.78 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
5.18 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
4.7037 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=1.08 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with ozone in the gas phase (Atkinson \& Carter 1984) $\mathrm{k}_{\mathrm{O} 3}=9.3 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=7.3 \mathrm{~d}$, based on rate constant $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.1.14.1
Reported vapor pressures of 1 -decene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1a) |
| :--- | :--- | :--- |
| (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| (3) |  |  |
| (4) |  |  |

Stull 1947
Forziati et al. 1950
Zwolinski \& Wilhoit 1971
summary of literature data

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :---: | :---: |
| 14.7 | 133.3 |
| 40.3 | 666.6 |
| 53.7 | 1333 |
| 67.8 | 2666 |
| 83.3 | 5333 |


| ebulliometry |  |
| :---: | ---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 86.774 | 6397 |
| 91.308 | 7694 |
| 95.134 | 8997 |
| 98.604 | 10334 |
| 101.844 | 11723 |


| selected values |  |
| :--- | ---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 54.40 | 1333 |
| 67.80 | 2666 |
| 76.33 | 4000 |
| 82.71 | 5333 |
| 87.875 | 6666 |

TABLE 2.1.2.1.14.1 (Continued)

| Stull 1947 |  | Forziati et al. 1950 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 93.5 | 7999 | 106.223 | 13848 | 92.236 | 7999 |
| 14.7 | 133.3 | 86.774 | 6397 | 54.40 | 1333 |
| 106.5 | 13332 | 111.213 | 16647 | 99.396 | 10666 |
| 126.7 | 26664 | 116.283 | 19950 | 105.198 | 13332 |
| 149.2 | 53329 | 120.995 | 23463 | 116.342 | 19998 |
| 192.0 | 101325 | 127.265 | 28990 | 124.760 | 26664 |
|  |  | 140.063 | 43759 | 131.607 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | 147.265 | 53710 | 137.421 | $39997$ |
|  |  | 154.939 | 66810 | 147.024 | $53329$ |
|  |  | 169.134 | 97662 | 154.861 | 66661 |
|  |  | 169.762 | 99247 | 161.533 | 79993 |
|  |  | 170.345 | 100747 | 163.376 | 93326 |
|  |  | 171.012 | 102487 | 168.464 | 95992 |
|  |  | 171.605 | 104026 | 170.052 | 98659 |
|  |  |  |  | 170.570 | 101325 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  | A | 6.96036 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | B | 1501.872 | A | 6.96034 |
|  |  | C | 197.578 | B | 1501.872 |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 170.570 | C | 197.578 |
|  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 170.570 |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /$ | $\left.\mathrm{ol}^{-1}\right)=$ |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 38.66 |
|  |  |  |  | at bp | 50.46 |



FIGURE 2.1.2.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for 1-decene.

### 2.1.2.2 Dienes

### 2.1.2.2.1 1,3-Butadiene



Common Name: 1,3-Butadiene
Synonym: $\alpha, \gamma$-butadiene, bivinyl, divinyl, erythrene, vinylethylene, biethylene, pyrrolylene
Chemical Name: 1,3-butadiene
CAS Registry No: 106-99-0
Molecular Formula: $\mathrm{C}_{4} \mathrm{H}_{6} ; \mathrm{CH}_{2}=\mathrm{CHCH}=\mathrm{CH}_{2}$
Molecular Weight: 54.091
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-108.91 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
-4.41 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.6211,0.6149\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, at saturation pressure, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$87.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987; Wang et al. 1992 Ruelle \& Kesselring 1997)
81.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
7.98 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
48.62, 45.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
735 (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$113857^{*} \quad\left(-1.50^{\circ} \mathrm{C}\right.$, static method-manometer, measured range -75.5 to $-1.50^{\circ} \mathrm{C}$, Heisig 1933)
336200* (calculated-Antoine eq. regression, temp range -102.8 to $4.6^{\circ} \mathrm{C}$, Stull 1947)
280600 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.85941-935.53 /\left(239.55+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -66 to $46^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
281000* (extrapolated-Antoine eq., temp range -58.201 to $14.43^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
280644 (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84999-930.546 /\left(238.854+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -58.201 to $14.43^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
61295* (20.211 ${ }^{\circ} \mathrm{C}$, temp range -16.204 to $33.257^{\circ} \mathrm{C}$, Boublikova 1972 ; quoted, Boublik et al. 1984)
247700 (extrapolated-Antoine eq., temp range -82.5 to $9.7^{\circ} \mathrm{C}$, Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 7761.0 /(\mathrm{T} / \mathrm{K})]+8.997505$; temp range -82.5 to $9.7^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 281650, 281510* (static method quartz manometer, measured range $15-55^{\circ} \mathrm{C}$, Flebbe et al. 1982)
281230, 310400(extrapolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.86369-1313.687 /\left(275.492+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -81 to $-24^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.97484-931.996 /\left(239.329+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -75 to $-1.5^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03555-998.106 /\left(245.233+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -87 to $-62^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
$\log (\mathrm{P} / \mathrm{mmHg})=6.84999-930.546 /\left(238.854+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -58 to $15^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
281000 (interpolated-Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16045-998.106 /(-27.916+\mathrm{T} / \mathrm{K})$; temp range 193-213 K (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.97489-930.546 /(-34.306+\mathrm{T} / \mathrm{K})$; temp range $213-276 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.99667-940.687 /(-33.017+\mathrm{T} / \mathrm{K})$; temp range $270-318 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.31615-1130.927 /(-5.606+\mathrm{T} / \mathrm{K})$; temp range $315-382 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.86984-3877.451 /(315.612+\mathrm{T} / \mathrm{K})$; temp range $380-425 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=30.0572-1.9891 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.2922 \cdot \log (\mathrm{~T} / \mathrm{K})+2.5664 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+5.1334 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $164-425 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$\ln (\mathrm{P} / \mathrm{atm})=9.16107-2154.139 /(\mathrm{T} / \mathrm{K}-33.596)$; temp range 207-319 K (Antoine eq., Oliveira \& Uller 1996)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
7460 (calculated-P/C, Mackay \& Shiu 1981)
6370 (calculated-1/ $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{w}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975; quoted, Howard 1989)
7150, 6230 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
10820 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
7720 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
1.99 (shake flask-GC, Leo et al. 1975; Hansch \& Leo 1979)
1.87, 1.68, 1.90 (calculated-fragment const., Rekker 1977)
2.22 (calculated-UNIFAC, Banerjee \& Howard 1988)
1.99 (recommended, Sangster 1989)
1.56 (calculated- $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
1.28 (calculated-K $\mathrm{K}_{\mathrm{ow}}$, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
1.86-2.36 (soils and sediments, calculated- $\mathrm{K}_{\mathrm{Ow}}$ and S , Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization: volatilizes rapidly from water and land (Howard 1989).
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, * data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}=8.4 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299 K (Japer et al. 1974)
$\mathrm{k}_{\mathrm{OH}}=(46.4 \pm 9.3) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=4.64 \times 10^{10} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}, \mathrm{t}_{1 / 2}=0.25 \mathrm{~h}$ for reaction with OH radical only, $\mathrm{t}_{1 / 2}=0.24 \mathrm{~h}$ with an average conen of 0.1 ppm of $\mathrm{O}_{3}$ at 300 K (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.9 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Atkinson \& Pitts, Jr. 1977)
$\mathrm{k}_{\mathrm{OH}}^{*}=(6.85 \pm 0.69) \times 10^{-11} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 299.5 K , measured range $299.9-424 \mathrm{~K}$ (flash photolysisresonance fluorescence, Atkinson et al. 1977)
$\mathrm{k}_{\mathrm{OH}}=6.9 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1979; quoted, Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{O} 3}{ }^{*}=(1.17 \pm 0.19) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K , measured range $276-324 \mathrm{~K}$ with atmospheric lifetime $\tau \sim 24 \mathrm{~h}$ due to reaction with $\mathrm{O}_{3}$ and $\tau \sim 4 \mathrm{~h}$ with OH radical (Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=6.85 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm \mathrm{K}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=6.22 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (relative rate method, Ohta 1983)
$\mathrm{k}_{\mathrm{O} 3}=(6.1-8.4) \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. to 299 K (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{NO} 3}=(5.34 \pm 0.62) \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}=(3.1 \pm 0.3) \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{NO}_{2}$ at $295 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}=6.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=0.053 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=8.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=6.4 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 2}=3.1 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{NO}_{2}$, at room temp. (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}=6.65 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{NO} 3}=2.1 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (fast flow system/MS, Benter \& Schindler 1988)
$\mathrm{k}_{\mathrm{OH}} *=6.66 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{NO} 3}=(4.4 \pm 0.8) \times 10^{-14} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ at $296 \pm 1 \mathrm{~K}(\mathrm{FTIR}$, Andersson \& Ljungström 1989)
$\mathrm{k}_{\mathrm{OH}}=66.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=7.5 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson 1990)
$\mathrm{k}_{\mathrm{NO} 3}=1.0 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=6.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=7.5 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Sabljic \& Gusten 1990)
$\mathrm{k}_{\mathrm{OH}}=2.6 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.0 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3} *=6.3 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.98 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis: will hydrolyze appreciably (Howard 1989).
Biodegradation: $\mathrm{t}_{1 / 2}($ aerobic $)=7 \mathrm{~d}, \mathrm{t}_{1 / 2}($ anaerobic $)=28 \mathrm{~d}$ in natural waters (Capel \& Larson 1995)
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: estimated photooxidation $t_{1 / 2}=0.24-24 \mathrm{~h}$ (Darnall et al 1976) for the reaction with hydroxyl radical; photooxidation with OH radicals with an estimated $\mathrm{t}_{1 / 2} \sim 3.1 \mathrm{~h}$ (Lyman et al. 1982; quoted, Howard 1989);
completely degraded within 6 h in a smog chamber irradiated by sunlight (Kopcynski et al 1972; quoted, Howard 1989);
$\mathrm{t}_{1 / 2}=15 \mathrm{~h}$ in air for the reaction with nitrate radical (Atkinson et al. 1984a; quoted, Howard 1989);
$\mathrm{t}_{1 / 2}=0.76-7.8 \mathrm{~h}$, based on measured photooxidation rate constants in air (Howard et al. 1991).
Surface water: $\mathrm{t}_{1 / 2}=1200$ to 48000 h , based on measured photooxidation rate constants with OH radicals in water
(Güsten et al. 1981; quoted, Howard et al. 1991);
estimated $t_{1 / 2}=3.8 \mathrm{~h}$ for evaporation from a model river 1 m deep with a $1 \mathrm{~m} / \mathrm{s}$ current and a $3 \mathrm{~m} / \mathrm{s}$ wind (Lyman et al. 1982; quoted, Howard 1989);
$\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $\mathrm{t}_{1 / 2}=9 \times 10^{4}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals and $\mathrm{t}_{1 / 2}=9 \times 10^{4} \mathrm{~d}$ for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant of $1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes with singlet oxygen in aquatic system (Mill \& Mabey 1985);
volatilizes rapidly with a half-life estimated to be several hours (Howard 1989);
$t_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991)
$\mathrm{t}_{1 / 2}($ aerobic $)=7 \mathrm{~d}, \mathrm{t}_{1 / 2}($ anaerobic $)=28 \mathrm{~d}$ in natural waters (Capel \& Larson 1995).
Ground water: $\mathrm{t}_{1 / 2}=336-1344 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:
Soil: $t_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991). Biota:

TABLE 2.1.2.2.1.1
Reported vapor pressures of 1,3 -butadiene at various temperatures and the coefficients for the vapor pressure equations



FIGURE 2.1.2.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3-butadiene.

### 2.1.2.2.2 <br> 2-Methyl-1,3-butadiene (Isoprene)



Common Name: 2-Methyl-1,3-butadiene
Synonym: isoprene
Chemical Name: 2-methyl-1,3-butadiene
CAS Registry No: 78-79-5
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{8} ; \mathrm{CH}_{2}=\mathrm{C}\left(\mathrm{CH}_{3}\right) \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 68.118
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-145.9 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
34 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.6809,0.6759\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$100.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
4.92 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 38.68, 34.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
642 (shake flask-GC, McAuliffe 1966)
545* $\quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $20-60^{\circ} \mathrm{C}$, Pavlova et al. 1966)
610* (recommended best value, IUPAC Solubility Data Series, temp range $20-60^{\circ} \mathrm{C}$, Shaw 1989a)
530* (calculated-liquid-liquid equilibrium LLE data, temp range 293.2-313.2 K, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
53329* $\quad\left(15.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -79.8 to $32.6^{\circ} \mathrm{C}$, Stull 1947)
$66816^{*} \quad\left(22.5^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $16.8-34.8^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90335-1080.996 /\left(234.668+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $16.8-34.8^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
$3349^{*} \quad\left(-38.227^{\circ} \mathrm{C}\right.$, inclined-piston manometer, measured range -57.598 to $-38.227^{\circ} \mathrm{C}$, Osborn \& Douslin 1969)

73330 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine \& Mookerjee 1975)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90334-1080.996 /\left(234.67+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -35 to $84^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
73300 (interpolated-Antoine eq., temp range -18.477 to $55.36^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
73340* (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88564-1071.578 /\left(233.513+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -18.477 to $55.36^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
73000, 78380 (calculated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.05468-1095.41 /\left(236.322+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -58 to $-38.2^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.05329-1092.997 /\left(236.002+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -16 to $33^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

73350 (interpolated-Antoine eq., temp range -52 to $-24^{\circ} \mathrm{C}$, Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01187-1126.159 /\left(238.88+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -52 to $-24^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) $\log (\mathrm{P} / \mathrm{mmHg})=6.88564-1071.518 /\left(233.51+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -19 to $55^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 73350 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.13677-1126,159 /(-34.266+\mathrm{T} / \mathrm{K})$; temp range $221-254 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.01-54-1071.578 /(-39.637+\mathrm{T} / \mathrm{K})$; temp range $254-316 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
73330, 10770 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
7840 (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
6230, 6520 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
7780 (calculated-P/C, Mackay \& Shiu 1981)
14940 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
7780 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
2.05 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
1.91 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
2.06 (calculated-measured $\gamma^{\circ}$ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}=16.5 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (chemiluminescence, Adeniji et al. 1981)
$\mathrm{k}_{\mathrm{O} 3} *=1.25 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in air at 296 K , measured range 278-323 K (static system-chemiluminescence, Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(9.26 \pm 1.5) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299 K , measured range $299-422 \mathrm{~K}$ (flash photolysisresonance fluorescence, Kleindienst et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=10.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm \mathrm{K}, \mathrm{k}_{\mathrm{OH}}($ calc $)=9.40 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (relative rate method, Ohta 1983)
$\mathrm{k}_{\mathrm{O} 3} *=(0.58-1.25) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ between $260-296 \mathrm{~K}$ (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{O} 3}=1.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.8 \mathrm{~d}^{-1}, \mathrm{k}_{\mathrm{OH}}=9.6 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $8 \mathrm{~d}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=5.8 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $12 \mathrm{~d}^{-1}$ (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{NO} 3}=(3.23 \pm 0.38) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}=(10.3 \pm 0.3) \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{NO}_{2}$ at $295 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=1.2 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=9.6 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=3.2 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}=10.2 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{OH}}=9.98 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, 9.26 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 299 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=(101 \pm 2) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $23.7 \pm 0.5^{\circ} \mathrm{C}$ (Edney et al. 1986)
$\mathrm{k}_{\mathrm{NO} 3}=1.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Benter \& Schindler 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=1.01 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=1.01 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=1.43 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=5.91 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.01 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}^{*}=6.78 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}} *=1.01 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}^{*}=6.78 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3} *=12.8 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=3.5 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: calculated atmospheric lifetimes: 32 h due to reaction with $\mathrm{O}_{3}$ in 24-h period, 2.9 h with OH radical during daytime, and 3.6 h for $\mathrm{NO}_{3}$ radical during nighttime for "clean atmosphere"; 10 h for reaction with $\mathrm{O}_{3}$ in 24-h period, 1.4 h with OH radical during daytime, and 22 min with $\mathrm{NO}_{3}$ radical during nighttime in "moderately polluted atmosphere" (Atkinson et al.1984a, Winer et al. 1984);
atmospheric lifetimes are calculated to be 28.3 h for the reaction with $\mathrm{O}_{3}, 2.9 \mathrm{~h}$ with OH radicals and 0.083 h with $\mathrm{NO}_{3}$ radicals, all based on the reaction rate constants with $\mathrm{O}_{3}, \mathrm{OH}$ and $\mathrm{NO}_{3}$ radicals in the gas phase (Atkinson \& Carter 1984)
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant of $1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes with singlet oxygen in aquatic system (Mill \& Mabey 1985).

## TABLE 2.1.2.2.2.1

Reported aqueous solubilities of 2-methyl-1,3-butadiene (isoprene) at various temperatures

| Pavlova et al. 1966 |  | Shaw 1989a |  | Góral et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | IUPAC tentative values |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 20 | 544.8 | 20 | 540 | 20 | 530 |
| 40 | 664.6 | 25 | 610 | 25 | 530 |
| 50 | 760.9 | 40 | 660 | 40 | 530 |
| 60 | 867.1 | 50 | 760 |  |  |
|  |  | 60 | 870 |  |  |



FIGURE 2.1.2.2.2.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 2-methyl-1,3-butadiene.

## TABLE 2.1.2.2.2.2

Reported vapor pressures of 2-methyl-1,3-butadiene (isoprene) at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |
| $\log \mathrm{P}=\mathrm{A}[1-\Phi /(\mathrm{T} / \mathrm{K})]$ | (5) where $\log \mathrm{A}=\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}$ |  |

1. 

| Stull 1947 |  | Forziati et al. 1950 |  | Osborn \& Douslin 1969 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | inclined-piston manometer |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  |  |  |  |  |  | liquid |
| -79.8 | 133.3 | 16.836 | 53718 | -57.598 | 842.86 | -51.561 | 1333 |
| -62.3 | 666.6 | 22.506 | 66816 | -55.186 | 1017 | -41.587 | 2666 |
| -53.3 | 1333 | 28.061 | 83780 | -52.77 | 1221 | -35.413 | 4000 |
| -43.5 | 2666 | 33.006 | 97665 | -50.35 | 1460 | -30.714 | 5333 |
| -32.6 | 5333 | 33.469 | 99260 | -47.93 | 1738 | -26.917 | 6666 |
| -25.4 | 7999 | 33.903 | 100757 | -45.507 | 2060 | -23.710 | 7999 |
| -16.0 | 13332 | 34.399 | 102484 | -43.083 | 2432 |  | liquid |
| -1.2 | 26664 | 34.834 | 104030 | -40.656 | 2860 | -18.447 | 10666 |
| 15.4 | 53329 |  |  | -38.227 | 3349 | -14.181 | 13332 |
| 32.6 | 101325 | Antoine eq. |  |  |  | -5.98 | 19998 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | Cox eq. |  | 0.221 | 26664 |
|  | -146.7 | A | 6.90335 | eq. 5 | P/atm | 5.268 | 33331 |
|  |  | B | 1080.996 | $\Phi$ | 307.217 | 9.557 | 39997 |
|  |  | C | 234.668 | a | 0.820543 | 16.646 | 53329 |

TABLE 2.1.2.2.2.2 (Continued)

| Stull 1947 |  | Forziati et al. 1950 |  | Osborn \& Douslin 1969 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | inclined-piston manometer |  | selected values |  |
| $t^{\circ}{ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\prime}{ }^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 34.067 | -b $\times 10^{-4}$ | 8.31178 | 22.437 | 66661 |
|  |  | $-b \times 10^{-7}$ |  | 10.32622 | 27.371 | 79993 |
|  |  | 31.693 |  |  | 93326 |
|  |  | 32.499 |  |  | 95992 |
|  |  | 33.287 |  |  | 98659 |
|  |  | 34.059 |  |  | 101325 |
|  |  | bp/ $/{ }^{\circ} \mathrm{C}$ |  |  | 34.059 |
|  |  | eq. 2 |  |  | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | A |  |  | 6.88654 |
|  |  | B |  |  | 1071.578 |
|  |  | C |  |  | 233.513 |
|  |  | for temp |  |  | - $18-55^{\circ} \mathrm{C}$ |
|  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ} \mathrm{mo}$ |  |  |  |
|  |  | at $25^{\circ} \mathrm{C}$ |  |  | 26.44 |
|  |  | at bp |  |  | 26.07 |

2. 

| Boublikova $\mathbf{1 9 7 2}$ (thesis) |  |
| :--- | :---: |
| in Boublik et al. $\mathbf{1 9 8 4}$ |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| -16.204 | 12046 |
| -12.508 | 14549 |
| -8.291 | 17921 |
| -4.649 | 21314 |
| -0.541 | 25780 |
| 2.793 | 29923 |
| 6.725 | 35493 |
| 10.416 | 41470 |
| 14.852 | 49704 |
| 20.211 | 61295 |
| 26.339 | 77125 |
| 33.257 | 98578 |
| bp $/{ }^{\circ} \mathrm{C}$ | 34.036 |
| eq. 2 | $\mathrm{P} / \mathrm{kPa}$ |
| A | 6.05329 |
| B | 1092.997 |
| C | 236.002 |



FIGURE 2.1.2.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1,3-butadiene.

### 2.1.2.2.3 2,3-Dimethyl-1,3-butadiene



Common Name: 2,3-Dimethyl-1,3-butadiene
Synonym:
Chemical Name: 2,3-dimethyl-1,3-butadiene
CAS Registry No: 513-81-5
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{10} ; \mathrm{CH}_{2}=\left(\mathrm{CH}_{3}\right) \mathrm{C}\left(\mathrm{CH}_{3}\right)=\mathrm{CH}_{2}$
Molecular Weight: 82.143
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-76 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
$68.8 \quad$ (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$0.7267,0.7222 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ : 113.0, $113.7\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 125.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
327 (quoted, Hine \& Mookerjee 1975)
226 (calculated-fragment solubility constants, Wakita et al. 1986)
94.3, 226 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
19200 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02388-1220.88 /\left(225.9+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -6 to $116^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
20160 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.25005-1302.766 /\left(238.42+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0.04-68.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
20160 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.1197-1299.69 /\left(238.09+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-68.5^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
20150 (interpolated-Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.3266-1346.0 /(-30.15+\mathrm{T} / \mathrm{K})$; temp range $273-342 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=29.9755-2.5677 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.8544 \cdot \log (\mathrm{~T} / \mathrm{K})+2.2361 \times 10^{-10} .(\mathrm{T} / \mathrm{K})+2.4591 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$
temp range 197-526 K (vapor pressure eq., Yaws 1994)
Henry's Law Constant $\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right.$ at $\left.25^{\circ} \mathrm{C}\right)$ :
$4830 \quad$ (calculated- $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{w}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
5420, 6990 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
21100 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(1.25 \pm 0.05) \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K} ; \mathrm{k}_{\mathrm{OH}}($ calc $)=1.26 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$
(relative rate method, Ohta 1983)
$\mathrm{k}_{\mathrm{OH}}=1.22 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson 1985, 1989)
$\mathrm{k}_{\mathrm{NO} 3}=2.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Benter \& Shindler 1988)
$\mathrm{k}_{\text {OH }}=1.22 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.052 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=2.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=1.22 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=2.1 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3} *=26.5 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant $\mathrm{k}=1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill \& Mabey 1985).

### 2.1.2.2.4 1,4-Pentadiene



Common Name: 1,4-Pentadiene
Synonym:
Chemical Name: 1,4-pentadiene
CAS Registry No: 591-93-5
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{8} ; \mathrm{CH}_{2}=\mathrm{CHCH}_{2} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 68.118
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-148.2 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
26 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.6608,0.6557 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ : 103.1, $103.9\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density) 103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
6.14 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 49.41, $52 / 3$ (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
558 (shake flask-GC, McAuliffe 1966)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
105100* (interpolated-Antoine eq. regression, temp range -83.5 to $26.1^{\circ} \mathrm{C}$, Stull 1947)
63774* $\quad\left(20.669^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $14.7-26.7^{\circ} \mathrm{C}$ (Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84880-1025.016 /\left(232.354+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $14.7-26.7^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
97900 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine \& Mookerjee 1975)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84880-1025.016 /\left(232.354+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -41 to $72^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
3611* $\quad\left(-43.083^{\circ} \mathrm{C}\right.$, inclined-piston manometer, measured range -60.01 to $-43.083^{\circ} \mathrm{C}$, Osborn \& Douslin 1969)

98000 (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971; quoted, Mackay \& Shiu 1981)
97940* (derived from compiled data, temp range -57.16 to $26^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.83543-1017.995 /\left(231.461+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -33.271 to $46.73^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 6826.6 /(\mathrm{T} / \mathrm{K})]+7.899113$; temp range -83.5 to $26.1^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
98300, 99400 (extrapolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.06018-1063.485 /\left(236.447+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -78.84 to $-18.08^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.34694-1239.949 /\left(238.278+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -60.0 to $-26.05^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
97930 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.17401-1155.378 /\left(244.30+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -57 to $-37^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) $\log (\mathrm{P} / \mathrm{mmHg})=6.83543-1017.995 /\left(231.46+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -33 to $47^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) 97900 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.29891-1155.378 /(-28.852+\mathrm{T} / \mathrm{K})$; temp range $216-234 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.96033-1017.995 /(-41.698+\mathrm{T} / \mathrm{K})$; temp range $236-307 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=23.7408-2.0505 \times 10^{3} /(\mathrm{T} / \mathrm{K})-5.679 \cdot \log (\mathrm{~T} / \mathrm{K})-5.9671 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+1.1242 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $125-479 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
12140 (calculated $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
15640 (calculated-bond contribution, Hine \& Mookerjee 1975)
12000 (calculated-P/C, Mackay \& Shiu 1981)
13620 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
11946 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
2.48 (shake flask, Log P Database, Hansch \& Leo 1987)
2.48 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(50.6 \pm 1.3) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K} ; \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=50.2 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (relative rate method, Ohta 1983)
$\mathrm{k}_{\mathrm{OH}}=5.33 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson 1985, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=5.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{NO} 3}=7.8 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (fast flow system, Benter \& Shindler 1988)
$\mathrm{k}_{\mathrm{OH}}=5.3 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant $\mathrm{k}=1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.2.4.1
Reported vapor pressures of 1,4-pentadiene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  |
| $\log \mathrm{P}=\mathrm{P}-\mathrm{B}=\mathrm{A}-\mathrm{C}+\mathrm{C} /(\mathrm{C}+\mathrm{K})$ |  | (3) $\left.{ }^{\circ} \mathrm{C}\right)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ |  | (4) |  |
| $\log \mathrm{P}=\mathrm{A}[1-\Phi /(\mathrm{T} / \mathrm{K})]$ |  | (5) where $\log \mathrm{A}=\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}$ |  |




FIGURE 2.1.2.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-pentadiene.

### 2.1.2.2.5 1,5-Hexadiene



Common Name: 1,5-Hexadiene Synonym:
Chemical Name: 1,5-Hexadiene
CAS Registry No: 592-42-7
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{10} ; \mathrm{CH}_{2}=\mathrm{CH}\left(\mathrm{CH}_{2}\right)_{2} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 82.143
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-140.7 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
59.4 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
0.6920 (Weast 1984)
$0.6923,0.6878 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$119.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Wang et al. 1992)
125.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
169 (shake flask-GC, McAuliffe 1966)
$320 \quad\left(14^{\circ} \mathrm{C}\right.$, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
27730 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00740-1184.99 /\left(227.7+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -13 to $102^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
32077* $\quad\left(26.95^{\circ} \mathrm{C}\right.$, static method-Hg manometer, measured range $26.95-46.13^{\circ} \mathrm{C}$, Letcher \& Marsicano 1974)

29690 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.5741-1013.5 /\left(214.8+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $0-59^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
29670, 29690 (interpolated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.7368-1032.0 /(-56.15+\mathrm{T} / \mathrm{K})$; temp range 273-333 K (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.98314-1159.908 /(-40.998+\mathrm{T} / \mathrm{K})$; temp range 299-333 K (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=10.5886-2.0106 \times 10^{3} /(\mathrm{T} / \mathrm{K})+0.28813 \cdot \log (\mathrm{~T} / \mathrm{K})-9.562 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+7.164 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $132-507 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
13620 (calculated $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{w}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
17550, 23130 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
17150 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
$2.40 \quad$ (calculated $-\pi$ substituent constant, Hansch et al. 1968)
2.29 (calculated-MCI $\chi$, Murray et al. 1975)
2.45 (calculated-fragment const., Yalkowsky \& Morozowich 1980)
2.68 (calculated-hydrophobicity const., Iwase et al. 1985)
2.80 (recommended, Sangster 1989)
2.8208 (calculated-UNIFAC group contribution, Chen et al. 1993)
2.78 (calculated-f const., Müller \& Klein 1992)
2.43 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
2.75 (recommended, Sangster 1993)
2.73 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=6.16 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1983)
$\mathrm{k}_{\text {OH }}=6.35 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, 5.85 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with 1,3 -butadiene and propylene as standard substances respectively at $297 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1983)
$\mathrm{k}_{\mathrm{OH}}=6.2 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant of $1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.2.5.1
Reported vapor pressures of 1,5 -hexadiene at various temperatures
Letcher \& Marsicano 1974

| static method-Hg manometer |  |
| :--- | :---: |
| $\mathbf{t}{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 26.95 | 32077 |
| 28.93 | 34690 |
| 31.62 | 38530 |
| 34.54 | 43036 |
| 36.94 | 47169 |
| 39.96 | 52622 |
| 41.77 | 56022 |
| 43.04 | 58622 |
| 46.13 | 65221 |

Antoine eq.
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$

|  | $\mathrm{P} / \mathrm{mmHg}$ |
| :---: | :---: |
| A | 6.6228 |
| B | 1037.35 |
| C | -55.52 |



FIGURE 2.1.2.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 1,5-hexadiene.

### 2.1.2.2.6 1,6-Heptadiene

N

Common Name: 1,6-Heptadiene
Synonym:
Chemical Name: 1,6-heptadiene
CAS Registry No: 3070-53-9
Molecular Formula: $\mathrm{C}_{7} \mathrm{C}_{12}$
Molecular Weight: 96.170
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -129 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
$90 \quad$ (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.714
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$134.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Wang et al. 1992)
148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
44.0 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
Henry's Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
2.90 (calculated $-\pi$ substituent constants, Hansch et al. 1968)
2.73 (calculated-MCI $\chi$, Murray et al. 1975)
3.31 (calculated-fragment const., Müller \& Klein 1992)
2.85 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.2189 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constant and Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant of $1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill \& Mabey 1985).

### 2.1.2.3 Alkynes

### 2.1.2.3.1 1-Butyne



Common Name: 1-Butyne
Synonym: ethyl acetylene, but-1-yne
Chemical Name: 1-butyne
CAS Registry No: 107-00-6
Molecular Formula: $\mathrm{C}_{4} \mathrm{H}_{6}, \mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{C} \equiv \mathrm{CH}$
Molecular Weight: 54.091
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ :
-125.7 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 8.08 (Lide 2003)

Density (g/cm ${ }^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.650. $0.65\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, at saturation pressure, Dreisbach 1959)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$83.22 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 81.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 6.03 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 40.9, 36.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
2870 (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations): $\log (\mathrm{P} / \mathrm{mmHg})=6.97497-986.46 /\left(232.85+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -67 to $43^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
188251 (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.07338-1101.71 /\left(235.81+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -30.8 to $26.8^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 6596.9 /(\mathrm{T} / \mathrm{K})]+8.032581$; temp range -92.5 to $8.7^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) $\log (\mathrm{P} / \mathrm{mmHg})=6.98198-988.75 /\left(233.01+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -68 to $27^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 ) 188220 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.10688-988.75 /(-40.14+\mathrm{T} / \mathrm{K})$; temp range $205-289 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=43.8278-2.4255 \times 10^{3} /(\mathrm{T} / \mathrm{K})-14.141 \cdot \log (\mathrm{~T} / \mathrm{K})+8.2138 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+7.4889 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $147-443 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
1880 (calculated $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{w}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
2210, 1800 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
1910 (calculated-P/C, Mackay \& Shiu 1981)
2820 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
1846 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
1.44, 1.48 (quoted, calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=1.79 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (static system-IR, Dillemuth et al. 1963)
$\mathrm{k}_{03}=(33 \pm 5) \times 10^{-21} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 1 \mathrm{~K}$ (static system-UV, DeMore 1971)
$\mathrm{k}_{\mathrm{O} 3}=(19.7 \pm 2.6) \times 10^{-21} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al.1984b)
$\mathrm{k}_{\mathrm{OH}}^{*}=(10.42 \pm 1.38) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K , measured range $253-343 \mathrm{~K}$ (discharge flowresonance fluorescence, Boodaghians et al. 1987)
$\mathrm{k}_{\mathrm{OH}}=8.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=8.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=2.0 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{03}=1.79 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K ; and $1.79 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, 4.0 \times 10^{-21} \mathrm{~cm}^{3}$ molecule $^{-1}$ $\mathrm{s}^{-1}$ at 294 K (literature review, Atkinson 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:

### 2.1.2.3.2 $\quad$ 1-Pentyne



Common Name: 1-Pentyne
Synonym: pent-1-yne
Chemical Name: 1-pentyne
CAS Registry No: 627-19-0
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{8} ; \mathrm{CH} \equiv \mathrm{C}\left(\mathrm{CH}_{2}\right)_{2} \mathrm{CH}_{3}$
Molecular Weight: 68.118
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-90 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
40.1 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.6901,0.6849\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
98.71, $99.46\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, calculated-density)
103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
1570 (shake flask-GC, McAuliffe 1966)
1049 (generator column-GC, Tewari et al. 1982a,b)
1363 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
57520 (calculated from determined data, Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97263-1095.42 /\left(227.53+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -50 to $70^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)
57600 (interpolated-Antoine eq., temp range -33 to $61^{\circ} \mathrm{C}$ Zwolinski \& Wilhoit 1971)
57462 (derived from compiled data, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04614-1092.52 /\left(227.18+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -33 to $61^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)

57540 (interpolated-Antoine eq., temp range -44 to $61^{\circ} \mathrm{C}$, Dean 1985)
$\log (\mathrm{P} / \mathrm{mmHg})=6.96734-1092.52 /\left(227.18+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -44 to $61^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
57540 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.09224-1092.52 /(-45.97+\mathrm{T} / \mathrm{K})$; temp range $229-315 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=33.8369-2.4684 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.4301 \cdot \log (\mathrm{~T} / \mathrm{K})+6.1345 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+4.676 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $167-481 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
2536 (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
2980, 2660 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
2500 (calculated-P/C, Mackay \& Shiu 1981)
3422 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
4983 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
1.98 (shake flask-UV, Hansch et al. 1968, Hansch \& Anderson 1967)
2.12 (generator column-GC, Tewari et al. 1982a,b)
1.98 (recommended, Sangster 1989, 1993)
1.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(11.17 \pm 0.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $253-343 \mathrm{~K}$ (discharge flowresonance fluorescence, Boodaghians et al. 1987, quoted, Atkinson 1989)
$\mathrm{k}_{\mathrm{NO} 3}=7.54 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (Atkinson 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:

### 2.1.2.3.3 1-Hexyne



Common Name: 1-Hexyne
Synonym: hex-1-yne
Chemical Name: 1-hexyne
CAS Registry No: 693-02-7
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{10} ; \mathrm{C}_{4} \mathrm{H}_{9} \mathrm{C} \equiv \mathrm{CH}$
Molecular Weight: 82.143
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-131.9 (Dreisbach 1959; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
71.33 (Dreisbach 1959)
71.3 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.7155,0.7155 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$114.8\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
125.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
360 (shake flask-GC, McAuliffe 1966)
686 (generator column-GC, Tewari et al. 1982a,b)
688 (generator column-GC, Miller et al. 1985)
392 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
18140 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91212-1194.6 /\left(225.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -8 to $118^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

18145 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.03702-1194.6 /(-48.15+\mathrm{T} / \mathrm{K})$; temp range $265-391 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=55.7231-3.2541 \times 10^{3} /(\mathrm{T} / \mathrm{K})-18.405 \cdot \log (\mathrm{~T} / \mathrm{K})+9.5814 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+9.2278 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 141-516 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
4020 (calculated-1/ $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
4210, 4020 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
4310 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
2166 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
2.48 (calculated- $\pi$ substituent constants, Hansch et al. 1968)
2.73 (generator column-GC, Tewari et al. 1982a,b)
2.73 (recommended, Sangster 1989, 1993)
2.73 (selected, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(12.6 \pm 0.04) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $253-343 \mathrm{~K}$ (discharge flowresonance fluorescence, Boodaghians et al. 1987; quoted, Atkinson 1989)
$\mathrm{k}_{\mathrm{NO} 3}=1.60 \times 10^{-15} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (Atkinson 1991)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:

### 2.1.2.3.4 1-Heptyne



Common Name: 1-Heptyne
Synonym:
Chemical Name: 1-heptyne
CAS Registry No: 628-71-7
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{12}$
Molecular Weight: 96.170
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -81 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
99.7 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$0.7330 \quad$ (Weast 1984)
$0.7328,0.7283 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$131.2\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
94.0 (shake flask-GC, McAuliffe 1966)

107 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
7000 (Antoine eq., Dreisbach 1959)
4298 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.27249-1314.492 /\left(208.097+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $63.1-99.98^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
7500 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.4039-1392.4 /(-56.55+\mathrm{T} / \mathrm{K})$; temp range $336-373 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=38.1255-3.064 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.679 \cdot \log (\mathrm{~T} / \mathrm{K})+1.2244 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+3.668 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $154-537 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
6830 (calculated-1/ $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
5950, 6090 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
5420 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
7160 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
2.98 (calculated- $\pi$ substituent constants, Hansch et al. 1968)
2.93 (calculated-MCI $\chi$, Murray et al. 1975)
2.98 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
2.99 (calculated-fragment const., Müller \& Klein 1992)
3.18 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 2.1.2.3.5 1-Octyne



Common Name: 1-Octyne
Synonym:
Chemical Name: 1-octyne
CAS Registry No: 629-05-0
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{14} ; \mathrm{C}_{6} \mathrm{H}_{13} \mathrm{C} \equiv \mathrm{CH}$
Molecular Weight: 110.197
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-79.3 (Dreisbach 1959; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): $127-128$
126.3 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.7461,0.7419 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$147.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
170.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
24.0 (shake flask-GC, McAuliffe 1966)
25.4 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
1813 (calculated-Antoine eq., Dreisbach 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=7.02447-1413.8 /\left(215.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25-170^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

1723 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.36895-1997.558 /\left(202.608+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $69.2-271.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1715 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.19321-1427.434 /(-214.625+\mathrm{T} / \mathrm{K})$; temp range $84.8-126.26 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
8208 (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
8208, 9000 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
6827 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
8325 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
3.48 (calculated $\pi$ substituent constants, Hansch et al. 1968)
3.37 (calculated-MCI $\chi$, Murray et al. 1975)
3.49 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.52 (calculated-f const., Müller \& Klein 1992)
3.84 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

### 2.1.2.3.6 1-Nonyne



Common Name: 1-Nonyne
Synonym:
Chemical Name: 1-nonyne
CAS Registry No: 3452-09-3
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{16} ; \mathrm{C}_{7} \mathrm{H}_{15} \mathrm{C} \equiv \mathrm{CH}$
Molecular Weight: 124.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-50 (Dreisbach 1959; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): $150-151$
150.8 (Dreisbach 1959; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.7570
(Weast 1984)
$0.7568,0.7527 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$164.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Ruelle \& Kesselring 1997)
192.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
7.20 (shake flask-GC, McAuliffe 1966)
6.30 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
835 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine \& Mookerjee 1975)
$\log (\mathrm{P} / \mathrm{mmHg})=6.77410-1404.7 /\left(210.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $50-223^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1959)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
14600 (calculated-1/ $\mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
11600, 13010 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
8700 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
14400 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {Ow }}$ :
3.98 (calculated- $\pi$ substituent constants, Hansch et al. 1968)
3.81 (calculated-MCI $\chi$, Murray et al. 1975)
3.98 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
4.05 (calculated-fragment const., Müller \& Klein 1992)
4.50 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

### 2.1.2.4 Cycloalkenes

### 2.1.2.4.1 Cyclopentene



Common Name: Cyclopentene
Synonym:
Chemical Name: cyclopentene
CAS Registry No: 142-29-0
Molecular Formula: $\mathrm{C}_{5} \mathrm{H}_{8}$
Molecular Weight: 68.118
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -135.0 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
44.2 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.7720,0.7665\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$88.2\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
92.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 27.92, $26.96 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $0.48,3.36 ; 3.84\left(-186.08,-135.05^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 29.83, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
535 (shake flask-GC, McAuliffe 1966)
611 (shake flask-titration with bromine, Natarajan \& Venkatachalam 1972) 1645 (shake flask-GC, Pierotti \& Liabastre 1972)
540 (suggested "tentative" value, IUPAC Solubility Data Series, Shaw 1989a)
719 (calculated-liquid-recommended liquid equilibrium LLE data, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
$39890^{*} \quad\left(19.77^{\circ} \mathrm{C}\right.$, static method-quartz spiral gauge, measured range -42.75 to $19.77^{\circ} \mathrm{C}$, Lister 1941)
$43375^{*} \quad\left(21.028^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $11.3-45.024^{\circ} \mathrm{C}$, Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92066-1121.818 /\left(233.446+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $11.3-45.0^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Forziati et al. 1950)
50690 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92066-1121.818 /\left(233.446+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range -30 to $105^{\circ} \mathrm{C}$ (Antoine eq. for liquid state,
Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{atm})=[1-317.520 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.814441-7.42372 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+8.49035 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$
223.2-393.2 K (Cox eq., Chao et al. 1983)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92066-1121.818 /\left(223.45+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Dean 1985, 1992)
50710 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.01617-1105.926 /(-41.615+\mathrm{T} / \mathrm{K})$; temp range $249-318 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=30.1132-2.3537 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.0609 \cdot \log (\mathrm{~T} / \mathrm{K})-5.7786 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.4591 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $138-507 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
6370 (calculated $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{w}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
3580, 9650 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
6460 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
2957, $3408,3863,4372^{*}\left(10,15,20,25^{\circ} \mathrm{C}\right.$, headspace-GC, measured range $10-25^{\circ} \mathrm{C}$, Bakierowska \& Trzeszçzyñski 2003)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=6.989-1915 /(\mathrm{T} / \mathrm{K})$; temp range $10-25^{\circ} \mathrm{C}$, headspace-GC, Bakierowska \& Trzeszçzyñski 2003)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow: }}$ :
1.75 (calculated- $\pi$ substituent const., Hansch et al. 1968)
1.76 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
2.25 (calculated-fragment const., Müller \& Klein 1992)
2.1791 (calculated-UNIFAC group contribution, Chen et al. 1993)
2.80 (calculated-UNIFAC activity coeff., Dallos et al. 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=8.13 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Japar et al. 1974; quoted, Adeniji et al. 1981)
$\mathrm{k}_{03}=9.69 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (chemiluminescence, Adeniji et al. 1981)
$\mathrm{k}_{\mathrm{O} 3}=(2.75 \pm 0.33) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 1 \mathrm{~K}$ (Atkinson et al. 1983a)
$\mathrm{k}_{\mathrm{OH}}=(6.39 \pm 0.23) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1983b)
$\mathrm{k}_{\mathrm{0} 3}=4.97 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 291.5 K in synthetic air (Bennett et al. 1987)
$\mathrm{k}_{\mathrm{0} 3}=(62.4 \pm 3.5) \times 10^{-17} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=4.99 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 3 \mathrm{~K}$, and $\mathrm{k}_{\mathrm{OH}}=5.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ relative to propene (relative rate method, Rogers 1989)
$\mathrm{k}_{\mathrm{OH}}=(5.02-6.73) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (literature review, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=4.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \mathrm{~K}, \mathrm{k}_{\mathrm{NO} 3}=4.6 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=6.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=5.81 \times 10^{-13} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{OH}}=6.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=5.3 \times 10^{-13} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}{ }^{*}=5.7 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: photooxidation rate constant of $4.97 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}_{3}$ in synthetic air was determined at atmospheric pressure at 291.5 K (Bennett et al. 1987);
rate constant $\mathrm{k}=4.99 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with OH radicals in air at 298 K (Rogers 1989).

Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals in aquatic system, and $\mathrm{t}_{1 / 2}=40 \mathrm{~d}$,
based on rate constant $\mathrm{k}=2 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the oxidation of cyclic olefins with singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.4.1.1
Reported vapor pressures and Henry's law constants of cyclopentene at various temperatures and the coefficients for the vapor pressure equations
$\begin{array}{lll}\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) & \text { (1) } & \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\ \log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) & \text { (2) } & \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) \\ \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K}) & \text { (3) } & \\ \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K}) & \text { (4) } \\ \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \cdot\left[\mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}\right] & \text { (5) } \\ \log (\mathrm{P} / \mathrm{atm})=\mathrm{A}^{\prime}\left[1-\left(\mathrm{T}_{\mathrm{B}} / \mathrm{T}\right)\right] & \text { (6) where } \log \mathrm{A}^{\prime}=\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}\end{array}$
Vapor pressure

| Lister 1941 |  | Forziati et al. 1950 |  | Bakierowska \& Trzeszçzyñski 2003 |
| :---: | :---: | :---: | :---: | :---: |
| static-quartz spiral gauge |  | ebulliometry |  | headspace-GC |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad$ Pa m ${ }^{\mathbf{~ m o l}}{ }^{\mathbf{- 1}}$ |
| -42.75 | 1447 | 11.325 | 28994 | 102957 |
| -24.18 | 4742 | 15.718 | 34940 | 15 3408 |
| 0 | 17292 | 21.028 | 43375 | 203863 |
| 19.77 | 39890 | 26.506 | 53710 | 254372 |
|  |  | 32.34 | 66807 |  |
|  |  | 39.678 | 93760 | $\ln \left(1 / \mathrm{K}_{\text {AW }}\right)=6.989-1915 /(\mathrm{T} / \mathrm{K})$ |
|  |  | 43.146 | 97653 |  |
|  |  | 43.624 | 99247 |  |
|  |  | 44.071 | 100744 |  |
|  |  | $44.576$ | $102469$ |  |
|  |  | $45.024$ | $104009$ |  |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 44.242 |  |
|  |  | Antoine eq. eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |
|  |  | A | $6.92066$ |  |
|  |  | B | 1121.818 |  |
|  |  | C | 233.446 |  |



FIGURE 2.1.2.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for cyclopentene.

### 2.1.2.4.2

Cyclohexene


Common Name: Cyclohexene
Synonym: 1,2,3,4-tetrahydrobenzene, tetrahydrobenzene
Chemical Name: cyclohexene
CAS Registry No: 110-83-8
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{10}$
Molecular Weight: 82.143
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -103.5 (Weast 1982-83; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 82.98 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.8110,0.8061\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959) $0.8102 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
101.4 (calculated-density, Stephenson \& Malanowski 1987; Ruelle \& Kesselring 1997)
110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 33.142, $30.485\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 29.125, $27.276\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 3.28 (Riddick et al. 1986)
$4.23,3.28 ; 7.51\left(-134.45,-104.45^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
49.85, 41.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):

```
130 (shake flask-cloud point, McBain & Lissant 1951)
160 (Farkas 1964)
213 (shake flask-GC, McAuliffe 1966)
299* (25.11 ' C, shake flask-GC, measured 5.11-45.21 }\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , Pierotti & Liabastre 1972)
281,286 (23.5}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , elution chromatography, Schwarz 1980)
160 (recommended best value, IUPAC Solubility Data Series, Shaw 1989a)
246* (calculated-liquid-liquid equilibrium LLE data, temp range 278.2-318.2 K, Góral et al. 2004)
```

Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$160,752,3345,8723^{*}\left(-44.42,-24.85,0.18 .45^{\circ} \mathrm{C}\right.$, static method-quartz spiral gauge, Lister 1941)
$11734^{*} \quad\left(24.794^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $12.2-83.9^{\circ} \mathrm{C}$ (Forziati et al. 1950)
$\log (\mathrm{P} / \mathrm{mmHg})=6.888617-1229.973 /\left(224.104+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $12.2-83.9^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
11840 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88617-1229.973 /\left(224.104+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $3.0-146^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$19885^{*} \quad\left(36.875^{\circ} \mathrm{C}\right.$, comparative ebulliometry, measured range $36.875-91.378^{\circ} \mathrm{C}$, Meyer \& Hotz 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=[1-356.172 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.873674-9.73841 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+10.9078 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $213.2-364.53 \mathrm{~K}$ (Cox eq., Chao et al. 1983)

11800 (selected lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=7.109-2289.0 /(\mathrm{T} / \mathrm{K})$; temp range: not specified (Antoine eq., Riddick et al. 1986)
11850 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.997323-1221,899 /(-49.978+\mathrm{T} / \mathrm{K})$; temp range $309-385 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=52.1749-3.238 \times 10^{3} /(\mathrm{T} / \mathrm{K})-16.878 \cdot \log (\mathrm{~T} / \mathrm{K})+8.0388 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+1.3259 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $170-560 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated):
4020 (calculated $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
4946, 13310 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
4568 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
$3960 \quad\left(23^{\circ} \mathrm{C}\right.$, batch air stripping-IR, Nielsen et al. 1994)
2069, 2467, 2618, 2965 ( $10,15,20,25^{\circ} \mathrm{C}$, headspace-GC, Bakierowska \& Trzeszçzyñski 2003)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=5.860-1691 /(\mathrm{T} / \mathrm{K})$; temp range $10-25^{\circ} \mathrm{C}$, headspace-GC, Bakierowska \& Trzeszçzyñski 2003)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
2.16 (calculated- $\pi$ substituent constants, Hansch et al. 1968)
2.86 (shake flask-GC, Leo et al. 1975)
1.90 (shake flask-GC, Canton \& Wegman 1983)
2.86 (recommended, Sangster 1989, 1993)
2.86 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.92* $\quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\circ}$ in octanol, measured range $20.29-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997) 2.83 (calculated-measured $\gamma^{\infty}$ in pure octanol and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.20 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom (Herron \& Huie 1973)
$\mathrm{k}_{\mathrm{OH}}=6.77 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (relative rate method, Atkinson et al. 1979)
$\mathrm{k}_{\mathrm{O} 3}=1.69 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ at 298 K (Japar et al. 1974)
$\mathrm{k}_{\mathrm{O} 3}=2.04 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 2 \mathrm{~K}$ (chemiluminescence, Adeniji et al. 1981)
$\mathrm{k}_{\mathrm{O} 3}=(1.04 \pm 0.14) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 1 \mathrm{~K}$ (Atkinson et al. 1983a)
$\mathrm{k}_{\mathrm{OH}}=(6.43 \pm 0.17) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1983b)
$\mathrm{k}_{\mathrm{OH}}=(64.1 \pm 2.5) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ (relative rate method, Ohta 1983)
$\mathrm{k}_{\mathrm{O} 3}=1.04 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 297 K (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{O} 3}=1.04 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=6.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=0.29 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=21 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom and $\mathrm{k}_{\mathrm{NO} 2}<0.2 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$
$\mathrm{s}^{-1}$ with $\mathrm{NO}_{2}$ (Atkinson \& Aschmann 1984)
$\mathrm{k}_{\mathrm{O} 3}=1.51 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ in synthetic air at 295 K (Bennett et al. 1987)
$\mathrm{k}_{\mathrm{O} 3}=(7.8 \pm 0.5) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=5.40 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K and $\mathrm{k}_{\mathrm{OH}}=6.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ relative to propene (relative rate method, Rogers 1989)
$\mathrm{k}_{\mathrm{OH}}=6.77 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=6.77 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=5.3 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=6.75 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=5.3 \times 10^{-13} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=5.28 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (quoted, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=6.77 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}^{*}=5.9 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3}{ }^{*}=81.4 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals in aquatic system, and $\mathrm{t}_{1 / 2}=40 \mathrm{~d}$, based on rate constant $\mathrm{k}=2 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.4.2.1
Reported aqueous solubilities of cyclohexene at various temperatures

| Pierotti \& Liabastre 1972 |  | Shaw 1989a |  | Góral et al. 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC/FID |  | IUPAC "tentative" values |  | calc-recommended LLE data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 5.11 | 280 | 5 | - | 5.1 | 265 |
| 15.21 | 298.5 | 15 | - | 15.2 | 251 |
| 25.11 | 299 | 20 | - | 20 | 246 |
| 35.21 | 302.5 | 25 | 160 | 23.5 | 246 |
| 45.21 | 310.5 | 35 | - | 25 | 246 |
|  |  | 45 | - | 25.1 | 246 |
|  |  |  |  | 35.2 | 251 |
|  |  |  |  | 45.2 | 265 |



FIGURE 2.1.2.4.2.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for cyclohexene.

TABLE 2.1.2.4.2.2
Reported vapor pressures and octanol-air partition coefficients of cyclohexene at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{aligned}
& \log P=A-B /(T / K) \\
& \log P=A-B /\left(C+t /{ }^{\circ} \mathrm{C}\right) \\
& \log P=A-B /(C+T / K) \\
& \log P=A-B /(T / K)-C \cdot \log (T / K) \\
& \log P=A-B /(T / K)-C \cdot \log (T / K)+D \cdot\left[P /(T / K)^{2}\right] \\
& \log (P / a t m)=A^{\prime}\left[1-\left(T_{B} / T\right)\right]
\end{aligned}
$$

(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \quad$ (1a)
(2)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(3)
(6) where $\log \mathrm{A}^{\prime}=\mathrm{a}+\mathrm{bT}+\mathrm{cT}^{2}$

| Vapor pressure |  |  |  |  | $\log \mathrm{K}_{\mathrm{OA}}$Gruber et al. 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Lister 1941 | Forziati et al. 1950 |  | Meyer \& Hotz 1973 |  |  |  |
| static-quartz spiral gauge | ebulliometry |  | comparative ebulliometry |  | GC det'd activity coeff. |  |
| $\mathbf{t}{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -44.42 160 | 12.236 | 6417 | 36.875 | 19885 | 20.29 | 2.926 |
| -24.85 752 | 15.920 | 7709 | 43.560 | 26084 | 30.3 | 2.762 |
| $0 \quad 3345$ | 19.137 | 9006 | 49.795 | 33189 | 40.4 | 2.594 |
| 18.45 8723 | 22.063 | 10344 | 55.785 | 41404 | 50.28 | 2.447 |
|  | 24.794 | 11734 | 62.537 | 52551 |  |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)= 32.59 \\ & \text { at } 27^{\circ} \mathrm{C}\end{aligned}$ | 28.490 | 13858 | 68.815 | 64943 |  |  |
|  | 32.702 | 16651 | 75.354 | 80213 |  |  |
|  | 36.996 | 19958 | 81.075 | 95764 |  |  |
|  | 40.976 | 23358 | 86.112 | 111325 |  |  |
|  | 46.302 | 28995 | 91.378 | 129633 |  |  |
|  | 51.191 | 35060 |  |  |  |  |
|  | 57.107 | 43376 | bp/ ${ }^{\circ} \mathrm{C}$ | 82.945 |  |  |
|  | 63.200 | 53712 |  |  |  |  |
|  | 69.708 | 66808 | Antoine eq. |  |  |  |
|  | 76.766 | 83761 | $\text { eq. } 3$ | $\mathrm{P} / \mathrm{cmHg}$ |  |  |
|  | 81.757 | 97648 | A | 5.872420 |  |  |
|  | 82.292 | 99248 | B | 1221.899 |  |  |
|  | 82.791 | 100746 | C | 223.1720 |  |  |
|  | 83.353 | 102470 |  |  |  |  |
|  | 83.852 | 104010 | Cox eq. $\text { eq. } 6$ | P/atm |  |  |
|  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | a | 0.833958 |  |  |
|  | A | 6.88617 | $-\mathrm{b} \times 10^{3}$ | 0.742586 |  |  |
|  | B | 1229.973 | $\mathrm{c} \times 10^{6}$ | 0.767278 |  |  |
|  | C | $224.104$ | $\mathrm{T}_{\mathrm{B}} / \mathrm{K}$ | 356.0954 |  |  |
|  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | $82.979$ |  |  |  |  |



FIGURE 2.1.2.4.2.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexene.


FIGURE 2.1.2.4.2.3 Logarithm of $\mathrm{K}_{\mathrm{OA}}$ versus reciprocal temperature for cyclohexene.

### 2.1.2.4.3 1-Methylcyclohexene



Common Name: 1-Methylcyclohexene Synonym:
Chemical Name: 1-methylcyclohexene
CAS Registry No: 591-49-1
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{12}$
Molecular Weight: 96.170
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -120.4 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 110.3 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.8102,0.8058\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1959; Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$118.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
133.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $37.75,32.70\left(25^{\circ}\right.$, bp, Dreisbach 1955)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 6.63 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
43.16, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
52.0 (shake flask-GC, McAuliffe 1966)
64.1 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
4080 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.86861-1308.0 /\left(218.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25-165^{\circ} \mathrm{C}$, (Antoine eq. for liquid state, Dreisbach 1955)

3933 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.0101-1311.087 /(-56.045+\mathrm{T} / \mathrm{K})$; temp range $333-384 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$4858 \quad\left(25.25^{\circ} \mathrm{C}\right.$, transpiration method, Verevkin et al. 2000)
$\ln (\mathrm{P} / \mathrm{Pa})=23.65-4531 /(\mathrm{T} / \mathrm{K})$; temp range $275.4-313.4 \mathrm{~K}$ (transpiration method, Verevkin et al. 2000)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
7660 (calculated $-1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
7485, 14260 (calculated-group contribution, calculated-bond contribution, Hine \& Mookerjee 1975)
11070 (calculated-MCI $\chi$, Nirmalakhandan \& Speece 1988)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
1.05 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
2.20 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , and Half-Lives., $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=9.44 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 305 K (Darnall et al. 1976, Atkinson 1989)
$\mathrm{k}_{\mathrm{NO} 3}=(2.87 \pm 0.34) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}<0.20 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O} 3}=1.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=6.4 \times 10^{-11} \mathrm{~cm}^{3}$
molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{NO} 3}=2.9 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ;$ and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\left.\mathrm{O}{ }^{3} \mathrm{P}\right)$
atom at room temp. (relative rate method, Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}=9.45 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 294 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=9.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=9.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}{ }^{*}=1.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=1.65 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=9.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals in aquatic system, and $\mathrm{t}_{1 / 2}=40 \mathrm{~d}$, based on rate constant $\mathrm{k}=2 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill \& Mabey 1985).

### 2.1.2.4.4 Cycloheptene



Common Name: Cycloheptene
Synonym: suberene
Chemical Name: cycloheptene
CAS Registry No: 628-92-2
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{12}$
Molecular Weight: 96.170
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-56 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
115 (Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.8228 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$116.9 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Lande \& Banerjee 1981; Wang et al. 1992)
129.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $36.73 \quad\left(27^{\circ} \mathrm{C}\right.$, Lister 1941)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$5.28,0.71,0.97 ; 6.96\left(-119.15,-63.15,-56.15^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 42.14, 45.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
66.0 (shake flask-GC, McAuliffe 1966)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations): $188,821,2636,6547\left(-21.44,0,19.82,39.06^{\circ} \mathrm{C}\right.$, static method-quartz spiral gauge, Lister 1941) 2670 (interpolated-Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.27243-2011.9 /(\mathrm{T} / \mathrm{K})$; temp range $251-313 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
2.57 (calculated- $\pi$ substituent constants, Hansch et al. 1968)
2.75 (calculated-MCI $\chi$, Murray et al. 1975)
3.073 (calculated-UNIFAC group contribution, Chen et al. 1993)
2.58 (calculated-molar volume $\mathrm{V}_{\mathrm{M}}$, Wang et al. 1992)
3.37 (calculated-fragment const., Müller \& Klein 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:

```
\(\mathrm{k}_{03}=(3.19 \pm 0.36) \times 10^{-16} \mathrm{~cm}^{3}\) molecule \(^{-1} \mathrm{~s}^{-1}\) at \(297 \pm 1 \mathrm{~K}\) (Atkinson et al. 1983a; quoted, Atkinson \&
    Carter 1984)
\(\mathrm{k}_{\mathrm{OH}}=(7.08 \pm 0.11) \times 10^{-11} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}\) at 298 K (relative rate method, Atkinson et al. 1983b)
\(\mathrm{k}_{\mathrm{OH}}=7.44 \times 10^{-11} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}\) at 298 K (Atkinson et al. 1983b, Atkinson 1989)
\(\mathrm{k}_{03}=(28.3 \pm 1.5) \times 10^{-17} \mathrm{~cm}^{3}\) molecule \(^{-1} \mathrm{~s}^{-1}\) at \(297 \pm 2 \mathrm{~K}\) in a smog chamber (Nolting et al. 1988)
\(\mathrm{k}_{\mathrm{NO} 3}=2.80 \times 10^{-13} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=7.13 \times 10^{-11} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}\) at 298 K (Sabljic \& Güsten 1990)
\(\mathrm{k}_{\mathrm{NO} 3}=4.84 \times 10^{-13} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}\) at 298 K (Atkinson 1991)
\(\mathrm{k}_{\mathrm{OH}}=7.4 \times 10^{-11} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=4.8 \times 10^{-13} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}\), and \(\mathrm{k}_{\mathrm{O} 3} *=2.45 \times 10^{-16} \mathrm{~cm}^{3}\)
    molecule \({ }^{-1} \mathrm{~s}^{-1}\) at 298 K (recommended, Atkinson 1997)
```

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals in aquatic system, and $\mathrm{t}_{1 / 2}=40 \mathrm{~d}$, based on rate constant $\mathrm{k}=2 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill \& Mabey 1985).

### 2.1.2.4.5 <br> Cyclooctene



Common Name: Cyclooctene Synonym:
Chemical Name: cyclooctene
CAS Registry No: 931-87-3 (cis-octene), 931-89-5 (trans-octene)
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{14}$
Molecular Weight: 110.197
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-12, -59 (cis-, trans-cyclooctene, Weast 1982-83; Lide 2003)
-14.5 to $-15.5 \quad$ (cis-cyclooctene, Stephenson \& Malanowski 1987)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
138, 143 (cis-, trans-cyclooctene, Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.8472,0.8483 \quad\left(20^{\circ} \mathrm{C}\right.$, cis-, trans-cyclooctene, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
130.1 (cis-, $20^{\circ} \mathrm{C}$, calculated-density, McAuliffe 1966; Lande \& Banerjee 1981; Wang et al. 1992)
129.9 (trans-, $20^{\circ} \mathrm{C}$, calculated-density, McAuliffe 1966; Lande \& Banerjee 1981; Wang et al. 1992)
146.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$41.57 \quad\left(27^{\circ} \mathrm{C}\right.$, Lister 1941)
Enthalpy of Sublimation, $\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
22.9* (generator column-GC/FID, measured range 273.15-313.15 K, Dohányosová et al. 2004)
$\ln x=-33.3561+20.8640 / \tau+43.2804 \cdot \ln \tau, \tau=[(\mathrm{T} / \mathrm{K}) / 298.15]$, temp range $273.15-313.15 \mathrm{~K}$ (generator columnGC/FID, Dohányosová et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
209.3, 774.6, 2333, $5948\left(0,19.83,40.36,60.22^{\circ} \mathrm{C}\right.$, static method-quartz spiral manometer, Lister 1941)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.3641-2194.3 /(\mathrm{T} / \mathrm{K})$, temp range $273-441 \mathrm{~K}$ (cis-cyclooctene, Antoine eq., Stephenson \& Malanowski 1987)
1010 (interpolated from data of Lister 1941, temp range 273.15-313.15 K, Dohányosová et al. 2004)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$. Additional data at other temperatures designated * are compiled at the end of this section.):
4842* (derived from measured mole fraction solubility and solute fugacity, temp range 273.15-313.15 K, Dohányosová et al. 2004)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :

Environmental Fate Rate Constants, $k$ and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}{ }^{*}=3.75 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (cis-cyclooctene, recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:

TABLE 2.1.2.4.5.1
Reorted aqueous solubilities and Henry's law constants of cyclooctene at various temperatures

| Aqueous solubility |  |  |  | Henry's law constant |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Dohányosová et al. 2004 |  |  |  | Dohányosová et al. 2004 |  |
| generator column-GC/FID |  | smoothed raw exptl data |  | from solute fugacity $f$ and $x$ |  |
| T/K | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
|  | raw data |  |  |  |  |
| 274.15 | 20.39 | 273.15 | 19.9 | 273.15 | 1184.4 |
| 274.15 | 20.14 | 278.15 | 20.2 | 278.15 | 1625.4 |
| 278.15 | 20.39 | 283.15 | 20.7 | 283.15 | 2196 |
| 278.15 | 19.59 | 288.15 | 21.3 | 288.15 | 2898 |
| 283.15 | 21.24 | 293.15 | 22.0 | 293.15 | 3780 |
| 283.15 | 20.45 | 298.15 | 22.9 | 298.15 | 4842 |
| 288.15 | 20.94 | 303.15 | 23.9 | 303.15 | 6120 |
| 288.15 | 20.63 | 308.15 | 25.1 | 308.15 | 7614 |
| 293.15 | 21.92 | 313.15 | 26.5 | 313.15 | 9378 |
| 298.15 | 23.63 |  |  |  |  |
| 298.15 | 24.61 | $\ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau$ |  |  |  |
| 303.15 | 22.84 | $\tau=\mathrm{T} / 298.15$ |  |  |  |
| 303.15 | 23.14 | A | -33.3561 |  |  |
| 308.15 | 27.24 | B | 20.8640 |  |  |
| 308.15 | 24.73 | C | 23.4396 |  |  |
| 308.15 | 26.88 |  |  |  |  |
| 313.15 | 27.31 |  |  |  |  |
| 313.15 | 24.80 |  |  |  |  |



FIGURE 2.1.2.4.5.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for cyclooctene.


FIGURE 2.1.2.4.5.2 Logarithm of Henry's law constant versus reciprocal temperature for cyclooctene.

### 2.1.2.4.6 <br> 1,4-Cyclohexadiene



Common Name: 1,4-Cyclohexadiene
Synonym: 1,4-dihyrobenzene
Chemical Name: 1,4-cyclohexadiene
CAS Registry No: 628-41-1
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{8}$
Molecular Weight: 80.128
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-49.2 (Weast 1983-83; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
85.5 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
0.8471 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$93.60 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
103.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $0.82,5.72 ; 6.53$ ( $-81.15,-49.15^{\circ} \mathrm{C}$, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
29.16, 38.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
700 (shake flask-GC, McAuliffe 1966)
930* (shake flask-GC, measured range $5.11-45.21^{\circ} \mathrm{C}$, Pierotti \& Liabstre 1972)
800* (recommended, temp range $5-45^{\circ} \mathrm{C}$, IUPAC Solubility Data Series, Shaw 1989a)
979* (calculated-liquid-liquid equilibrium LLE data, temp range 278.3-318.4 K, Góral et al. 2004)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
11892* ( $31.1^{\circ} \mathrm{C}$, static method- Hg manometer, measured range $304.25-322.23 \mathrm{~K}$, Letcher \& Marsicano 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=[1-368.566 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.916704-6.81678 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})-7.02362 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $304.25-322.23 \mathrm{~K}$ (Cox eq., Chao et al. 1983)
8973 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.86553-1176.707 /\left(214.528+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $31.1-49.08^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
9009 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.41736-1475.149 /(-26.108+\mathrm{T} / \mathrm{K})$; temp range: 304-360 K (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$
2.30 (shake flask, Log P Database, Hansch \& Leo 1987)
2.48 (calculated-UNIFAC activity coeff., Banerjee \& Howard 1988)
2.30 (recommended, Sangster 1989, 1993)
2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{03}=(0.639 \pm 0.074) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 1 \mathrm{~K}$ (Atkinson et al. 1983a)
$\mathrm{k}_{\mathrm{OH}}=(9.48 \pm 0.39) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1983b)
$\mathrm{k}_{\mathrm{NO} 3}=(2.89 \pm 0.035) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{O} 3}=63.9 \times 10^{-18} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=9.5 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=0.29 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $^{-1}$ $\mathrm{s}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 2}<0.4 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{NO}_{2}$ (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=9.90 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ calc $)=1.03 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{NO} 3}=7.8 \times 10^{-13} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K (fast flow system, Benter \& Schindler 1988)
$\mathrm{k}_{\mathrm{OH}}=(99.2-99.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (review, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=9.91 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{NO} 3}=5.30 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{NO}_{3}$ radical at nights (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=6.6 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=9.95 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=6.6 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3}{ }^{*}=4.6 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Surface water: $\mathrm{t}_{1 / 2} \sim 320 \mathrm{~h}$ and $9 \times 10^{4} \mathrm{~d}$ for oxidation by OH and $\mathrm{RO}_{2}$ radicals for olefins in aquatic system, and $\mathrm{t}_{1 / 2}=19 \mathrm{~h}$, based on rate constant $\mathrm{k}=1.0 \times 10^{7} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill \& Mabey 1985).

TABLE 2.1.2.4.6.1
Reported aqueous solubilities of 1,4-cyclohexadiene at various temperatures

| Aqueous solubility |  |  |  |  |  | Vapor pressure |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Pierotti \& Liabastre 1972 |  | Shaw 1989a |  | Góral et al. 2004 |  | Letcher \& Marsicano 1974 |
| shake flask-GC/FID |  | IUPAC "tentative" values |  | calc-recommended LLE data |  | static method-Hg manometer |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | T/K S/g.m ${ }^{\mathbf{3}}$ |
| 5.11 | 851.9 | 5 | 900 | 5.1 | 1068 | 304.2511892 |
| 15.21 | 958.5 | 15 | 900 | 15.2 | 979 | 307.6713826 |
| 25.11 | 936.2 | 25 | 800 | 25.0 | 979 | 310.7615812 |
| 35.21 | 963.4 | 35 | 1000 | 25.1 | 979 | 312.9242655 |
| 45.21 | 1010 | 45 | 1000 | 35.2 | 979 | 316.6720238 |
|  |  |  |  | 45.2 | 1068 | 319.9422998 |
|  |  |  |  |  |  | $322.23 \quad 25251$ |
|  |  |  |  |  |  | Antoine eq., $\quad \mathrm{P} / \mathrm{mmHg}$ $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ |
|  |  |  |  |  |  | A 7.2687 |
|  |  |  |  |  |  | B $\quad 1461.75$ |
|  |  |  |  |  |  | C $\quad-29.4$ |



FIGURE 2.1.2.4.6.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,4-cyclohexadiene.

### 2.1.2.4.7 <br> Cycloheptatriene



Common Name: Cycloheptatriene
Synonym: tropilidene
Chemical Name: 1,3,5-cycloheptatriene
CAS Registry No: 544-25-2
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{8}$
Molecular Weight: 92.139
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-79.5 (Weast 1982-83; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
117 (Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.8875 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$103.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Lande \& Banerjee 1981; Wang et al. 1992) 114.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$2.35,1.16 ; 3.51 \quad\left(-93.15,-75.15^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
21.11, 38.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
620 (shake flask-GC, McAuliffe 1966)
$669^{*} \quad\left(25.11^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $5.11-40.21^{\circ} \mathrm{C}$, Pierotti \& Liabastre 1972)
640* (recommended best value, temp range $5-45^{\circ} \mathrm{C}$, IUPAC Solubility Data Series, Shaw 1989)
563* (calculated-liquid-liquid equilibrium LLE data, temp range 278.3-318.4 K, Góral et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
3136* (ebulliometry, measured range $0-65^{\circ} \mathrm{C}$, Finke et al. 1956)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97032-1374.065 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+220.538\right.$ ); temp range $0-65^{\circ} \mathrm{C}$ (Antoine eq., ebulliometry, Finke et al. 1956)
2825, 3138 (interpolated-Antoine eq-I, II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.09522-1374.656 /(-52.612+\mathrm{T} / \mathrm{K})$; temp range $273-390 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.12574-1390.771 /(-53.069+\mathrm{T} / \mathrm{K})$; temp range $273-390 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
432 (calculated-P/C from selected data)
466 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
2.63 (shake flask, Eadsforth \& Moser 1983)
3.03 (HPLC-RT correlation, Eadsforth \& Moser 1983)
2.63 (recommended, Sangster 1989)
2.63 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=(5.39 \pm 0.078) \times 10^{-17} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=(9.12 \pm 0.23) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for at $294 \pm 2$ K (Atkinson et al. 1984b)
$\mathrm{k}_{03}=5.39 \times 10^{-17} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ for at 294 K (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{OH}}=9.74 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 294 K (Atkinson 1985)
$\mathrm{k}_{\mathrm{NO} 3}=1.18 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{OH}}=9.44 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{OH}}=96.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 294 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{NO} 3}=1.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (quoted, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}}=9.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3}=5.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:

## TABLE 2.1.2.4.7.1

Reported aqueous solubilities and vapor pressures of cycloheptatriene at various temperatures

| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |  |

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

$$
\begin{align*}
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1a}\\
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) \tag{2a}
\end{align*}
$$

Vapor pressure

| Pierotti \& Liabastre 1972 |  | Shaw 1989a |  | Góral et al. 2004 |  | Finke et al. 1956 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | IUPAC recommended |  | calc-recommended LLE data |  | ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 5.11 | 580.9 | 5 | 580 | 5.1 | 614 | 0 | 733.3 |
| 10.21 | 664.5 | 15 | 660 | 15.2 | 614 | 15 | 1815 |
| 25.11 | 669.4 | 25 | 640 | 25.0 | 563 | 20 | 2400 |
| 30.21 | 741.8 | 35 | 740 | 25.1 | 563 | 25 | 3136 |
| 40.21 | 764.8 | 45 | 760 | 35.2 | 614 | 30 | 4058 |
|  |  |  |  | 45.2 | 614 | 35 | 5198 |
|  |  |  |  |  |  | 40 | 6591 |
|  |  |  |  |  |  | 45 | 8286 |
|  |  |  |  |  |  | 50 | 10327 |
|  |  |  |  |  |  | 55 | 12774 |
|  |  |  |  |  |  | 60 | 15672 |
|  |  |  |  |  |  | 65 | 19094 |

TABLE 2.1.2.4.7.1 (Continued)

| Aqueous solubility |  |  |  |  |  | Vapor pressure |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Pierotti \& Liabastre 1972 |  | Shaw 1989a |  | Góral et al. 2004 |  | Finke et al. 1956 |  |
| shake flask-GC |  | IUPAC recommended |  | calc-recommended LLE data |  | ebulliometry |  |
| $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| $\begin{array}{cr} \mathrm{bp} /{ }^{\circ} \mathrm{C} & 115.60 \\ \Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ} \mathrm{~mol} & -1) \\ & =38.70 \\ \text { at } 25^{\circ} \mathrm{C} \end{array}$ |  |  |  |  |  |  |  |
|  |  |  |  |  |  | $\begin{gathered} \text { eq. } 2 \\ \text { A } \\ \text { B } \\ \text { C } \end{gathered}$ | $\begin{gathered} \mathrm{P} / \mathrm{mmHg} \\ 6.97032 \\ 1374.656 \\ 220.538 \end{gathered}$ |



FIGURE 2.1.2.4.7.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for cyclohepta-triene.


FIGURE 2.1.2.4.7.2 Logarithm of vapor pressure versus reciprocal temperature for cycloheptatriene.

### 2.1.2.4.8 <br> dextro-Limonene [(R)-(+)-Limonene]



Common Name: $d$-Limonene
Synonym: $d$ - $p$-mentha-1,8,-diene, (R)-(+)-p-mentha-1,8-diene, (+)-1-methyl-4-(1-methylethenyl)cyclohexene, $p$ -mentha-1,8-diene, carvene, cinene, citrene, cajeputene, kautschin
Chemical Name: dextro-limonene, (R)-(+)-limonene
CAS Registry No: 5989-27-5
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{16}$
Molecular Weight: 136.234
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-74 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
178 (Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $25^{\circ} \mathrm{C}$ ): 0.8403, $0.8383\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $162.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
192.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $45.1 \quad\left(25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
13.49 (shake flask-GC, Massaldi \& King 1973)
13.8 (selected lit., Riddick et al. 1986)
20.44 (shake flask-GC/FID, Fichan et al. 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
275.64 (calculated-Antoine eq. regression, Stull 1947)
275.5 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10508.4 /(\mathrm{T} / \mathrm{K})]+8.016262$; temp range $14.0-175^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$2670 \quad\left(68.2^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
278, 202 (calculated-Antoine eq.-I, II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.81591-2075.62 /(-16.65+\mathrm{T} / \mathrm{K})$; temp range $287-448 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.67098-2494.342 /(\mathrm{T} / \mathrm{K})$; temp range $288-323 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=9.3771-2.8246 \times 10^{3} /(\mathrm{T} / \mathrm{K})+1.0584 \cdot \log (\mathrm{~T} / \mathrm{K})-8.9107 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+4.8462 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 199-660 K (vapor pressure eq., Yaws 1994)
213 (activity coefficient-GC, Fichan et al. 1999)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
2725 (calculated-P/C from selected data)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.38 (RP-HPLC-RT correlation, Griffin et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated * data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=9 \times 10^{10} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$, with $\mathrm{t}_{1 / 2}<0.24 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(9.0 \pm 1.35) \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at 1 atm and $305 \pm 2 \mathrm{~K}$ (relative rate method, Winer et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=9.0 \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=3.9 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(6.50 \pm 0.52) \times 10^{10} \mathrm{~cm}^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Winer et al. 1976)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=13.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.(14.0,14.2) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1983b)
$\mathrm{k}_{\mathrm{NO} 3}=(7.7 \pm 1.7) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate technique, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{O} 3}=6.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes $\tau=6 \mathrm{~min}$ and 11 min in 24-h in clean and moderately polluted atmosphere, respectively; $\mathrm{k}_{\mathrm{OH}}=1.42 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=2.0 \mathrm{~h}$ and 1.0 h during daytime in clean and moderately polluted atmosphere respectively, $\mathrm{k}_{\mathrm{NO} 3}=7.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=9 \mathrm{~min}$ and 0.9 min during nighttime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}<3.5 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for gas phase reaction with $\mathrm{NO}_{2}$ at 295 K (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=6.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=1.42 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=7.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=1.29 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=6.0 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $36 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=1.4 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $12 \mathrm{~d}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=1.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $290 \mathrm{~d}^{-1}$ (Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{O} 3}=6.0 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $36 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=1.7 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $7.3 \mathrm{~d}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=1.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $290 \mathrm{~d}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=(16.9 \pm 0.5) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al.1986)
$\mathrm{k}_{\mathrm{O} 3}=6.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=36 \mathrm{~min} ; \mathrm{k}_{\mathrm{OH}}=1.7 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\tau($ calc $)=1.6 \mathrm{~h}, \mathrm{k}_{\mathrm{NO} 3}=1.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\tau($ calc $)=5.0 \mathrm{~min}$ for clean tropospheric conditions at room temp. (Atkinson et al. 1986)
$\mathrm{k}_{\mathrm{OH}}=(146-171) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294-305 \mathrm{~K}$ (review, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=1.71 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.22 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=2.03 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=7.2 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}<.24 \mathrm{~h}$ in air based on its photooxidation rate constant of $9 \times 10^{13} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the gas phase reaction with hydroxyl radical (Darnall et al. 1976; Lloyd et al. 1976);
calculated lifetimes: $\tau=36 \mathrm{~min}$ due to reaction with $\mathrm{O}_{3}$ in $24-\mathrm{h}$ period, $\tau=2.0 \mathrm{~h}$ with OH radical during daytime, and $\tau=9 \mathrm{~min}$ for $\mathrm{NO}_{3}$ radical during nighttime for "clean" atmosphere; $\tau=11 \mathrm{~min}$ for reaction with $\mathrm{O}_{3}$ in 24-h period, $\tau=1.0 \mathrm{~h}$ with OH radical during daytime, and $\tau=0.9 \mathrm{~min}$ for $\mathrm{NO}_{3}$ radical during nighttime in moderately polluted atmosphere (Atkinson et al. 1984a);
calculated atmospheric lifetimes, $\tau=36 \mathrm{~min}, 1.6 \mathrm{~h}$ and 5.0 min for reaction with $\mathrm{O}_{3}, \mathrm{OH}$ and $\mathrm{NO}_{3}$ radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);
calculated tropospheric lifetimes $\tau=1.1 \mathrm{~h}, 1.9 \mathrm{~h}$ and 53 min due to reactions with OH radical, $\mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ radical, respectively, at room temp. (Corchnoy \& Atkinson 1990).

### 2.1.2.4.9 $\quad \alpha$-Pinene



Common Name: $\alpha$-Pinene Synonym: $d l$-pinene, 2-pinene
Chemical Name: 2,6,6-trimethylbicyclo[3,1,1]hept-2-ene
CAS Registry No: 7785-70-8
$\alpha$-pinene $d$-Form 80-56-8
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{16}$
Molecular Weight: 136.234
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):

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-55 (dl-Form, Weast 1982-83)
-64 (d-Form, Riddick et al. 1986; Lide 2003)
-50 (d-Form, Stephenson & Malanowski 1987)
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Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
156.2 (dl-Form, Weast 1982-83; Lide 2003)

156 (d-Form, Stephenson \& Malanowski 1987)
155-156 ( $d$-, l-Form, Budavari 1989)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ): $0.8582 \quad\left(20^{\circ} \mathrm{C}\right.$, $d l$-Form, Weast 1982-83) 0.8582, 0.8539 ( $d$-Form, Riddick et al. 1986) $0.8592,0.8591,0.8590\left(20^{\circ} \mathrm{C}, d l-, d-\right.$, $l$-Form, Budavari 1989)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
157.4 ( $d$-Form, Stephenson \& Malanowski 1987)
183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 46.61, $39.673 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
21.8, 3.42; 5.04 (quoted lit. values; shake flask-GC/FID, Fichan et al. 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
$640^{*}, 800 \quad\left(22.2,22.5^{\circ} \mathrm{C}\right.$, measured range $21.1-148^{\circ} \mathrm{C}$, Pickett \& Peterson 1929)
$237.3^{*} \quad\left(13.25^{\circ} \mathrm{C}, \mathrm{Hg}\right.$ manometer, measured range -6.0 to $13.25^{\circ} \mathrm{C}$, Linder 1931)
$666.6^{*} \quad\left(24.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -1.0 to $155.0^{\circ} \mathrm{C}$, Stull 1947)
457*, 655 (21.2, $27.2^{\circ} \mathrm{C}$, measured range $19.4-155.75^{\circ} \mathrm{C}$, Hawkins \& Armstrong 1954)
678 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9813.6 /(\mathrm{T} / \mathrm{K})]+7.898207$; temp range -1.0 to $155^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
667 (Verschueren 1983)
605, 587 (interpolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.37971-1692.803 /\left(231.558+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $21.1-148^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data of Pickett \& Peterson 1929, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.95174-1430.936 /\left(206.42+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $19.44-155.75^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data of Hawkins \& Armstrong 1954, Boublik et al. 1984)
655 (selected, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=25.52644-3134.525 /(\mathrm{T} / \mathrm{K})-6.16045 \cdot \log (\mathrm{~T} / \mathrm{K})($ Riddick et al. 1986 $)$
( $\alpha$-pinene $d$-Form, interpolated-Antoine eq., temp range $292-433 \mathrm{~K}$, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{kPa})=5.92666-1414.16 /(\mathrm{T} / \mathrm{K})($ Antoine eq., liquid, temp range $292-433 \mathrm{~K}$ ( $\alpha$-pinene $d$-Form, Stephenson \& Malanowski 1987)
588 (interpolated-Antoine eq., temp range $19-156^{\circ} \mathrm{C}$, Dean 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.8525-1446.4 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+208.0\right)$; temp range $19-156^{\circ} \mathrm{C}$ (Antoine eq., Dean 1992)
$\log (\mathrm{P} / \mathrm{mbar})=7.076588-1511.961 /[(\mathrm{T} / \mathrm{K})-57.730]$; temp range $365-430 \mathrm{~K}$ (vapor-liquid equilibrium (VLE)Fischer still, Reich \& Sanhueza 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=21.4735-2.7156 \times 10^{3} /(\mathrm{T} / \mathrm{K})-5.0076 \cdot \log (\mathrm{~T} / \mathrm{K})+2.8146 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-1.5389 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 209-632 K (vapor pressure eq., Yaws 1994)
$613,581,465 ; 529$ (quoted lit. values; deduced from exptl. determined activity coeff. at infinite dilution, Fichan et al. 1999)

Henry's Law Constant $\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right.$ at $25^{\circ} \mathrm{C}$ or indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section.):
0.194* $\quad\left(20^{\circ} \mathrm{C}\right.$, calculated from measured liquid-phase diffusion coefficients, measured range -10 to $20^{\circ} \mathrm{C}$, Zhang et al. 2003)
$\ln \left[\mathrm{H}^{\prime} /(\mathrm{M} / \mathrm{atm})\right]=-6.590+3800 /(\mathrm{T} / \mathrm{K})$; temp range $263-293 \mathrm{~K}$ (Zhang et al. 2003)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
$4.44((+)-\alpha$-pinene, RP-HPLC-RT correlation, Griffin et al. 1999)
$4.48((-)-\alpha$-pinene, RP-HPLC-RT correlation, Griffin et al. 1999)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants $\mathrm{k}_{\mathrm{O} 3}$ for reaction with $\mathrm{O}_{3}$, $\mathrm{k}_{\mathrm{OH}}$ with OH radical and $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical at $25^{\circ} \mathrm{C}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=(3.48 \pm 0.52) \times 10^{10} \mathrm{~cm}^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Winer et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=3.5 \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=2.0 \times 10^{5} \mathrm{M}^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(1.60 \pm 0.06) \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (Winer et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=32 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1} \mathrm{~s}^{-1} \mathrm{k}_{\mathrm{O} 3}=67 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{O} 3}{ }^{*}=(8.4 \pm 1.9) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K , measured range $276-324 \mathrm{~K}$, atmospheric lifetime $\tau$ $=3-4 \mathrm{~h}$ due to reaction with $\mathrm{O}_{3}$, and $\tau \sim 4 \mathrm{~h}$ due to reaction with OH radical (Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{OH}}^{*}=(6.01 \pm 0.82) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $298-422 \mathrm{~K}$ (flash photolysisresonance fluorescence, Kleindlenst et al. 1982)
$\mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=8.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=(7.6,5.5,6.01) \times 10^{-11} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1983b)
$\mathrm{k}_{\mathrm{OH}} *=60.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $298-422 \mathrm{~K}$ (Flash photolysis-resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)
$\mathrm{k}_{\mathrm{NO} 3}=(3.4 \pm 0.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{O} 3}=8.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes of 4.6 h and 1.4 h in 24-h in clean and moderately polluted atmosphere, respectively; $\mathrm{k}_{\mathrm{OH}}=6.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes of 4.6 h and 2.3 h during daytime in clean and moderately polluted atmosphere, respectively, $\mathrm{k}_{\mathrm{NO} 3}=3.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes of 20 min and 2 min during nighttime in clean and moderately polluted atmosphere respectively at room temp. (Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}<2.1 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for gas phase reaction with $\mathrm{NO}_{2}$ at 295 K (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=8.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=6.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=3.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=640 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ at room temp. (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=8 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $5 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=6.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $5 \mathrm{~d}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=6.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $130 \mathrm{~d}^{-1}$ (Atkinson \& Carter 1984) $\mathrm{k}_{\mathrm{OH}}=(5.45 \pm 0.32) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al.1986)
$\mathrm{k}_{\mathrm{O} 3}=8.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=5.6 \mathrm{~h} ; \mathrm{k}_{\mathrm{OH}}=5.5 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\tau($ calc $)=5.1 \mathrm{~h}, \mathrm{k}_{\mathrm{NO} 3}=6.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ with $\tau($ calc $)=11 \mathrm{~min}$ for clean tropospheric conditions at room temp. (Atkinson et al. 1986)
$\mathrm{k}_{\mathrm{O} 3}=(8.6 \pm 1.3) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}} *=5.37 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}} *=5.37 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=5.79 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3}=(8.4,8.6) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1990)
$\mathrm{k}_{\mathrm{OH}}=9.12 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{NO} 3}=5.75 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Müller \& Klein 1991)
$\mathrm{k}_{\mathrm{OH}}=5.32 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=5.79 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}^{*}=6.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{OH}} *=5.37 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}^{*}=6.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O} 3} *=86.6 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=3.2 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}}($ lit. $)=5.45 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}($ calc $)=8.5 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (quoted; calculatedQSAR, Peeters et al. 1999)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants $\left(\mathrm{k}_{1}\right.$ and $\left.\mathrm{k}_{2}\right)$ :
Half-Lives in the Environment:
Air: calculated lifetimes: $\tau=4.6 \mathrm{~h}$ due to reaction with $\mathrm{O}_{3}$ in 24-h period, $\tau=4.6 \mathrm{~h}$ with OH radical during daytime, and $\tau=20 \mathrm{~min}$ for $\mathrm{NO}_{3}$ radical during nighttime for clean atmosphere; $\tau=1.4 \mathrm{~h}$ for reaction with $\mathrm{O}_{3}$ in 24 -h period, $\tau=2.3 \mathrm{~h}$ with OH radical during daytime, and $\tau=2 \mathrm{~min}$ with $\mathrm{NO}_{3}$ radical during nighttime in moderately polluted atmosphere (Atkinson et al.1984a, Winer et al. 1984);
calculated atmospheric lifetimes of $5.6 \mathrm{~h}, 5.1 \mathrm{~h}$ and 11 min for reaction with $\mathrm{O}_{3}, \mathrm{OH}$ and $\mathrm{NO}_{3}$ radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);
calculated tropospheric lifetimes of $3.4 \mathrm{~h}, 4.6 \mathrm{~h}$ and 2.0 h due to reactions with OH radical, $\mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ radical respectively at room temp. (Corchnoy \& Atkinson 1990).

TABLE 2.1.2.4.9.1
Reported vapor pressures of $\alpha$-pinene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(4)
1.

| Pickett \& Peterson 1929 |  |  |  | Linder 1931 |  | Stull 1947 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Ramsay \& Young method |  |  |  | Hg manometer |  | summary of literature data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 21.2 | 533 | 134.9 | 57128 | -6.0 | 54.66 | -1.0 | 133 |
| 22.0 | 573 | 135.4 | 57608 | 1.0 | 96.0 | 24.6 | 666.6 |
| 22.2 | 640 | 138.5 | 63728 | 13.25 | 237.3 | 37.3 | 1333 |
| 22.5 | 800 | 138.8 | 64261 |  |  | 51.4 | 2666 |

Pickett \& Peterson 1929

Linder 1931
Hg manometer
Hg mana

$$
\begin{align*}
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) \tag{2}
\end{align*}
$$

1. 

(Continued)

TABLE 2.1.2.4.9.1 (Continued)

| Pickett \& Peterson 1929 |  |  |  | Linder 1931 |  | Stull 1947 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Ramsay \& Young method |  |  |  | Hg manometer |  | summary of literature data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathbf{C}$ | $\mathbf{P / P a}$ |
| 54.7 | 3040 | 139.8 | 65861 |  |  | 66.8 | 5333 |
| 55.3 | 3200 | 140.1 | 66794 |  |  | 76.8 | 7999 |
| 55.5 | 3306 | 140.5 | 67461 |  |  | 90.1 | 13332 |
| 77.4 | 7839 | 141.2 | 68794 |  |  | 110.2 | 26664 |
| 77.5 | 7906 | 141.3 | 69327 |  |  | 132.3 | 53329 |
| 77.7 | 7959 | 141.9 | 70394 |  |  | 155.0 | 101325 |
| 77.9 | 8026 | 147.0 | 80526 |  |  |  |  |
| 78.6 | 8253 | 148.0 | 83060 |  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -55 |
| 79.3 | 8519 |  |  |  |  |  |  |
| 79.6 | 8639 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 155-158 |  |  |  |  |
| 101.1 | 19625 |  |  |  |  |  |  |
| 102.8 | 20758 |  |  |  |  |  |  |
| 103.2 | 21025 |  |  |  |  |  |  |
| 103.5 | 21238 |  |  |  |  |  |  |
| 103.7 | 21371 |  |  |  |  |  |  |
| 103.8 | 21451 |  |  |  |  |  |  |
| 131.2 | 52196 |  |  |  |  |  |  |
| 132.3 | 53462 |  |  |  |  |  |  |
| 132.4 | 53862 |  |  |  |  |  |  |
| 132.5 | 53902 |  |  |  |  |  |  |
| 132.7 | 54089 |  |  |  |  |  |  |
| 132.9 | 54275 |  |  |  |  |  |  |
| 133.0 | 54755 |  |  |  |  |  |  |
| 133.1 | 54862 |  |  |  |  |  |  |
| 133.2 | 54995 |  |  |  |  |  |  |

2. 

Hawkins \& Armstrong 1954

| $\mathbf{H g}$ manometer |  |  |  |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 19.45 | 408.0 | 65.63 | 4858 | 95.27 | 16164 | 155.77 | 100601 |
| 21.3 | 457.3 | 66.54 | 5121 | 102.25 | 20717 | 155.76 | 100793 |
| 27.25 | 654.6 | 68.27 | 5554 | 105.9 | 23430 |  |  |
| 29.72 | 790.6 | 70.45 | 6073 | 106.76 | 24217 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 155.9 |
| 37.07 | 1201 | 75.1 | 7430 | 110.53 | 27438 |  |  |
| 46.92 | 2015 | 76.04 | 7698 | 113.5 | 30135 | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |
| 53.69 | 2832 | 77.12 | 8033 | 115.07 | 31795 | A | 26.40174 |
| 54.18 | 2877 | 79.75 | 8905 | 122.11 | 39478 | B | 3134.525 |
| 56.57 | 3234 | 84.71 | 10859 | 125.02 | 42963 | C | 6.16045 |
| 57.09 | 3309 | 86.23 | 11536 | 129.87 | 49509 | 155.77 | 100601 |
| 57.3 | 3393 | 88.42 | 12512 | 135.72 | 58678 |  |  |
| 62.28 | 4221 | 92.01 | 14299 | 147.48 | 80731 |  |  |



FIGURE 2.1.2.4.9.1 Logarithm of vapor pressure versus reciprocal temperature for $\alpha$-pinene.

## TABLE 2.1.2.4.9.2

Reported Henry's law constants of $\alpha$-pinene at various temperatures
Zhang et al. 2003
liquid-phase diffusion coefficient

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ |
| :--- | :---: |
| -10 | 0.0397 |
| 0 | 0.0618 |
| 10 | 0.113 |
| 20 | 0.194 |
| $\ln (\mathrm{kH} / \mathrm{atm})=$ | $\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| eq. 3 | $\mathrm{H}^{\prime} /(\mathrm{M} \mathrm{atm}$ |
|  | $-1)$ |
| A | -6.59 |
| B | 3800 |



FIGURE 2.1.2.4.9.2 Logarithm of Henry's law constant versus reciprocal temperature for $\alpha$-pinene.

### 2.1.2.4.10



Common Name: $\beta$-Pinene
Synonym: $\beta$-Pinene $d$, or nopinene; $\beta$-Pinene $l$, or 2(10)-pinene
Chemical Name: 6,6-dimethyl-2-methylene bicyclo[3,1,1]heptane
CAS Registry No: 19172-67-3
$\beta$-pinene $l$-Form 127-91-3
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{16}$
Molecular Weight: 136.234
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ :
-61.54 (l-Form, Riddick et al. 1986)
-50 (l-Form, Stephenson \& Malanowski 1987)
-61.5 (l-Form, Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
164-166, 162.4 ( $d$-Form, $l$-Form, Weast 1982-83)
166 (l-Form, Riddick et al. 1986; Lide 2003)
163 (l-Form, Stephenson \& Malanowski 1987)
165-166, 164-166, 162-163 (dl-, $d$-, l-Form, Budavari 1989)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ :
0.8654, $0.8694\left(20^{\circ} \mathrm{C}, d-\right.$, $l$-Form, Weast 1982-83)
$0.8667 \quad\left(25^{\circ} \mathrm{C}, l\right.$-Form, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
157.4 (l-Form, Stephenson \& Malanowski 1987)
183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
43.471, 40.208 ( $25^{\circ} \mathrm{C}$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
32.7, 6.27; 11.04 (quoted lit. values; shake flask-GC, Fichan et al. 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section.):
613* (Ramsay \& Young method, measured range $24.3-158.1^{\circ} \mathrm{C}$, Pickett \& Peterson 1929)
$666.6^{*} \quad\left(30.0^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $4.2-158.3^{\circ} \mathrm{C}$, Stull 1947)
$345^{*}, 447$ (23.06, $26.8^{\circ} \mathrm{C}$, measured range $18.71-165.91^{\circ} \mathrm{C}$, Hawkins \& Armstrong 1954)
501 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10235.8 /(\mathrm{T} / \mathrm{K})]+8.633424$; temp range $4.2-158.3^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
667 (Verschueren 1983)
395 (interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.02052-1509.944 /\left(210.05+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $18.71-165.9^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Hawkins \& Armstrong 1954, Boublik et al. 1984)
$610 \quad$ (selected, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=27.90258-3318.845 /(\mathrm{T} / \mathrm{K})-6.94263 \cdot \log (\mathrm{~T} / \mathrm{K})($ Riddick et al. 1986)
391 (l-Form, interpolated- Antoine eq., temp range 291-441K, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{kPa})=6.04993-1520.15 /(\mathrm{T} / \mathrm{K}+62.75)$; temp range $291-441 \mathrm{~K}(l$-Form, Antoine eq., liquid, Stephenson \& Malanowski 1987)

394 (interpolated-Antoine eq., Dean 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.8984-1511.7 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+210.2\right)$; temp range $19-156^{\circ} \mathrm{C}$ (Antoine eq., Dean 1992)
$\log (\mathrm{P} / \mathrm{mbar})=7.067997-1539.348 /[(\mathrm{T} / \mathrm{K})-59.937]$; temp range $364-439 \mathrm{~K}$ (vapor-liquid equilibrium (VLE)Fischer still, Reich \& Sanhueza 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=46.3728-3.9789 \times 10^{3} /(\mathrm{T} / \mathrm{K})-13.284 \cdot \log (\mathrm{~T} / \mathrm{K})-1.3113 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+3.4783 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $120-651 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ ):

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
4.16 (RP-HPLC-RT correlation, Griffin et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for second order gas-phase rate constants $\mathrm{k}_{\mathrm{OH}}, \mathrm{k}_{\mathrm{O} 3}$ and $\mathrm{k}_{\mathrm{NO} 3}$ for reactions with OH radicals, $\mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ radicals or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=42 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$, with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(4.06 \pm 0.61) \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at 1 atm and $305 \pm 2 \mathrm{~K}$ (relative rate method, Winer et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=4.1 \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O} 3}=2.2 \times 10^{4} \mathrm{M}^{-1} \mathrm{~s}^{-1}$; and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(1.51 \pm 0.06) \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom (Winer et al. 1976)
$\mathrm{k}_{\mathrm{O} 3}=30 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=65 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Gaffney \& Levine 1979)
$\mathrm{k}_{\mathrm{O} 3}=(2.1 \pm 0.5) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ with atmospheric lifetime $\tau \sim 13 \mathrm{~h}$ due to reaction with $\mathrm{O}_{3}$ and $\tau \sim 4 \mathrm{~h}$ due to reaction with OH radical (Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(7.76 \pm 1.1) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $297-423 \mathrm{~K}$ (flash photolysisresonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=5.1 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=(6.4,7.76) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1983b)
$\mathrm{k}_{\mathrm{NO} 3}=(1.4 \pm 0.3) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{O} 3}=2.1 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated lifetimes $\tau=18 \mathrm{~h}$ and 5.5 h in $24-\mathrm{h}$ in clean and moderately polluted atmosphere respectively; $\mathrm{k}_{\mathrm{OH}}=7.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=3.6 \mathrm{~h}$ and 1.8 h during daytime in clean and moderately polluted atmosphere, respectively; $\mathrm{k}_{\mathrm{NO} 3}=$ $1.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=50 \mathrm{~min}$ and 5 min during nightime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)
$\mathrm{k}_{\mathrm{NO} 2}=<2.4 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for gas phase reaction with $\mathrm{NO}_{2}$ at 295 K (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{O} 3}=2.1 \times 10^{-17} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=7.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=1.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$; and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=640 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at room temp. (Atkinson et al. 1984b)
$\mathrm{k}_{\mathrm{OH}}=(7.95 \pm 0.52) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al.1986)
$\mathrm{k}_{\mathrm{O} 3}=2.1 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with calculated $\tau=18 \mathrm{~h} ; \mathrm{k}_{\mathrm{OH}}=8.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\tau($ calc $)=3.5 \mathrm{~h}, \mathrm{k}_{\mathrm{NO} 3}=2.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\tau($ calc $)=28 \mathrm{~min}$ for clean tropospheric conditions at room temp. (Atkinson et al. 1986)
$\mathrm{k}_{\mathrm{NO} 3}=2.36 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1988)
$\mathrm{k}_{\mathrm{O} 3}=(1.4 \pm 0.2) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $297 \pm 2 \mathrm{~K}$ in a smog chamber (Nolting et al. 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=7.89 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}} *=7.89 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=2.36 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3}=(2.1 ; 1.4) \times 10^{-17}$ $\mathrm{cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1990)
$\mathrm{k}_{\mathrm{OH}}=5.62 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{NO} 3}=2.34 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Müller \& Klein 1991)
$\mathrm{k}_{\mathrm{OH}}=7.82 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=2.36 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, at 298 K (Sabljic \& Güsten 1990)
$\mathrm{k}_{\mathrm{NO} 3}=2.51 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1991)
$\mathrm{k}_{\mathrm{O} 3}=12.2 \pm 1.3 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $22 \pm 1^{\circ} \mathrm{C}$ (Grosjean et al. 1993)
$\mathrm{k}_{\mathrm{OH}} *=7.89 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=2.51 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O} 3} *=1.5 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=2.7 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom, at 298 K (recommended, Atkinson 1997)
$\mathrm{k}_{\mathrm{OH}, \text { lit }}=7.95 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}($ calc $)=6.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (quoted; calculated-QSAR, Peters et al. 1999)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:
Air: calculated lifetimes: $\tau=18 \mathrm{~h}$ due to reaction with $\mathrm{O}_{3}$ in $24-\mathrm{h}$ period, $\tau=3.6 \mathrm{~h}$ with OH radical during daytime, and $\tau=50 \mathrm{~min}$ for $\mathrm{NO}_{3}$ radical during nighttime for "clean" atmosphere; $\tau=5.5 \mathrm{~h}$ for reaction with $\mathrm{O}_{3}$ in 24 -h period, $\tau=1.8 \mathrm{~h}$ with OH radical during daytime, and $\tau=5 \mathrm{~min}$ with $\mathrm{NO}_{3}$ radical during nighttime hours in "moderately polluted" atmosphere (Atkinson et al.1984a, Winer et al. 1984);
calculated atmospheric lifetimes of $18 \mathrm{~h}, 3.5 \mathrm{~h}$ and 28 min for reaction with $\mathrm{O}_{3}, \mathrm{OH}$ and $\mathrm{NO}_{3}$ radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986);
calculated tropospheric lifetimes of $2.3 \mathrm{~h}, 1.1 \mathrm{~d}$ and 4.9 h due to reactions with OH radical, $\mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ radical respectively at room temp. (Corchnoy \& Atkinson 1990).

TABLE 2.1.2.4.10.1
Reported vapor pressures of $\beta$-pinene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \quad$ (1a)
1.

Pickett \& Peterson 1929
Ramsay \& Young method

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 24.3 | 453.3 | 94.7 | 13839 | 131.9 | 47809 | 4.2 | $\mathbf{P} / \mathbf{P a}$ |
| 24.5 | 480 | 95.1 | 14225 | 132.1 | 48329 | 30.0 | 666.3 |
| 24.7 | 520 | 95.7 | 14585 | 132.6 | 48889 | 42.3 | 1333 |
| 24.8 | 400 | 96.0 | 14705 | 132.9 | 49583 | 58.1 | 2666 |
| 25.0 | 613 | 96.2 | 14905 | 133.6 | 50623 | 71.5 | 5333 |
| 25.4 | 653 | 96.5 | 14905 | 133.9 | 50796 | 81.2 | 7999 |
| 53.5 | 2486 | 105.8 | 20825 | 154.7 | 91792 | 94.0 | 13332 |
| 54.0 | 2440 | 106.0 | 20998 | 154.9 | 92126 | 114.1 | 26664 |
| 54.4 | 2466 | 106.4 | 21305 | 155.2 | 92459 | 136.1 | 53329 |
| 54.6 | 2520 | 106.9 | 21665 | 156.2 | 94859 | 158.3 | 101325 |
| 55.0 | 2586 | 107.1 | 21812 | 158.0 | 100258 |  |  |
| 68.7 | 4680 | 108.2 | 21932 | 158.1 | 100926 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  |
| 68.9 | 4720 | 131.2 | 47529 |  |  |  | - |
| 69.1 | 4866 | 131.6 | 47929 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | $160.2-163.8$ |  |  |
| 70.9 | 5240 | 131.7 | 47929 |  |  |  |  |

(Continued)

TABLE 2.1.2.4.10.1 (Continued)
2.

Hawkins \& Armstrong 1954

|  | $\mathbf{H g}$ manometer |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  |
| 18.72 | 252.0 | 50.11 | 1644 | 81.23 | 6949 | 161.22 | 89634 |  |
| 20.05 | 284.0 | 52.32 | 1812 | 85.96 | 8266 | 165.8 | 100788 |  |
| 23.09 | 345.3 | 56.57 | 2268 | 85.86 | 9983 | 157.82 | 101194 |  |
| 26.82 | 446.6 | 56.94 | 2341 | 90.80 | 11346 |  |  |  |
| 29.45 | 517.3 | 58.86 | 2550 | 94.12 | 12828 | $\mathrm{bp} /{ }^{\circ} \mathbf{C}$ | 166.0 |  |
| 31.68 | 592.0 | 59.48 | 3056 | 97.33 | 15948 |  |  |  |
| 32.03 | 592.0 | 62.62 | 3084 | 103.41 | 19288 | eq .4 | $\mathrm{P} / \mathrm{mmHg}$ |  |
| 36.78 | 793.3 | 66.52 | 3534 | 108.81 | 24117 | A | 28.77768 |  |
| 37.09 | 803.9 | 68.75 | 4014 | 115.50 | 27972 | B | 3318.845 |  |
| 39.41 | 929.3 | 72.23 | 4677 | 125.33 | 33079 | C | 6.94243 |  |
| 41.34 | 1037 | 75.43 | 5384 | 131.39 | 39762 |  |  |  |
| 45.52 | 1289 | 78.59 | 6141 | 136.02 | 45106 |  |  |  |
| 49.41 | 1580 | 80.88 | 6810 | 149.55 | 65069 |  |  |  |



FIGURE 2.1.2.4.10.1 Logarithm of vapor pressure versus reciprocal temperature for $\beta$-pinene.

### 2.2 SUMMARY TABLES AND QSPR PLOTS

## TABLE 2.2.1

Summary of physical properties of aliphatic and cyclic hydrocarbons

| Compound | CAS no. | Molecular formula | Molecular weight, MW $\mathrm{g} / \mathrm{mol}$ | m.p. ${ }^{\circ} \mathrm{C}$ | b.p. ${ }^{\circ} \mathrm{C}$ | Fugacity ratio, $F$ at $25^{\circ} \mathrm{C}^{*}$ | $\begin{gathered} \text { Density, } \rho \\ \mathrm{g} / \mathrm{cm}^{3} \text { at } \\ 20^{\circ} \mathrm{C} \end{gathered}$ | Molar volume, $\mathrm{V}_{\mathrm{M}} \mathrm{cm}^{3} / \mathrm{mol}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  | MW/ $\rho$ at $20^{\circ} \mathrm{C}$ | Le Bas |
| Alkanes: |  |  |  |  |  |  |  |  |  |
| Isobutane (2-Methylpropane) | 75-28-5 | $\mathrm{C}_{4} \mathrm{H}_{10}$ | 58.122 | -159.4 | -11.73 | 1 | 0.5571 | 104.33 | 96.2 |
| 2,2-Dimethylpropane (Neopentane) | 463-82-1 | $\mathrm{C}_{5} \mathrm{H}_{12}$ | 72.149 | -16.4 | 9.48 | 1 | 0.5910 | 122.08 | 118.4 |
| $n$-Butane | 106-97-8 | $\mathrm{C}_{4} \mathrm{H}_{10}$ | 58.122 | -138.3 | -0.5 | 1 | 0.5786 | 100.45 | 96.2 |
| 2-Methylbutane (Isopentane) | 78-78-4 | $\mathrm{C}_{5} \mathrm{H}_{12}$ | 72.149 | -159.77 | 27.88 | 1 | 0.6193 | 116.50 | 118.4 |
| 2,2-Dimethylbutane | 75-83-2 | $\mathrm{C}_{6} \mathrm{H}_{14}$ | 86.175 | -98.8 | 49.73 | 1 | 0.6492 | 132.74 | 140.6 |
| 2,3-Dimethylbutane | 79-29-8 | $\mathrm{C}_{6} \mathrm{H}_{14}$ | 86.175 | -128.10 | 57.93 | 1 | 0.6616 | 130.25 | 140.6 |
| 2,2,3-Trimethylbutane | 464-06-2 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -24.6 | 80.86 | 1 | 0.6901 | 145.20 | 162.8 |
| $n$-Pentane | 109-66-0 | $\mathrm{C}_{5} \mathrm{H}_{12}$ | 72.149 | -129.67 | 36.06 | 1 | 0.6262 | 115.22 | 118.4 |
| 2-Methylpentane (Isohexane) | 107-83-5 | $\mathrm{C}_{6} \mathrm{H}_{14}$ | 86.175 | -153.6 | 60.26 | 1 | 0.6322 | 136.31 | 140.6 |
| 3-Methylpentane | 96-14-0 | $\mathrm{C}_{6} \mathrm{H}_{14}$ | 86.175 | -162.90 | 63.27 | 1 | 0.66431 | 129.72 | 140.6 |
| 2,2-Dimethylpentane | 590-35-2 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -123.7 | 79.2 | 1 | 0.6739 | 148.69 | 162.8 |
| 2,4-Dimethylpentane | 108-08-7 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -119.5 | 80.49 | 1 | 0.6727 | 148.95 | 162.8 |
| 3,3-Dimethylpentane | 562-49-2 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -134.4 | 86.06 | 1 | 0.6933 | 144.53 | 162.8 |
| 2,2,4-Trimethylpentane (Isooctane) | 540-84-1 | $\mathrm{C}_{8} \mathrm{H}_{18}$ | 114.229 | -107.3 | 99.22 | 1 | 0.6919 | 165.09 | 185.0 |
| 2,3,4-Trimethylpentane | 565-75-3 | $\mathrm{C}_{8} \mathrm{H}_{18}$ | 114.229 | -109.2 | 113.5 | 1 | 0.7191 | 158.85 | 185.0 |
| $n$-Hexane | 110-54-3 | $\mathrm{C}_{6} \mathrm{H}_{14}$ | 86.175 | -95.35 | 68.73 | 1 | 0.6593 | 130.71 | 140.6 |
| 2-Methylhexane (Isoheptane) | 591-76-4 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -118.2 | 90.04 | 1 | 0.6786 | 147.66 | 162.8 |
| 3-Methylhexane | 589-34-4 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -119.4 | 92 | 1 | 0.6871 | 145.83 | 162.8 |
| 2,2,5-Trimethylhexane | 3522-94-9 | $\mathrm{C}_{9} \mathrm{H}_{20}$ | 128.255 | -105.7 | 124.09 | 1 | 0.7072 | 181.36 | 207.2 |
| $n$-Heptane | 142-82-5 | $\mathrm{C}_{7} \mathrm{H}_{16}$ | 100.202 | -90.55 | 98.4 | 1 | 0.6837 | 146.56 | 162.8 |
| 2-Methylheptane | 592-27-8 | $\mathrm{C}_{8} \mathrm{H}_{18}$ | 114.229 | -109.02 | 117.66 | 1 | 0.698 | 163.65 | 185.0 |
| 3-Methylheptane | 589-81-1 | $\mathrm{C}_{8} \mathrm{H}_{18}$ | 114.229 | -120.48 | 118.9 | 1 | 0.7075 | 161.45 | 185.0 |
| $n$-Octane | 111-65-9 | $\mathrm{C}_{8} \mathrm{H}_{18}$ | 114.229 | -56.82 | 125.67 | 1 | 0.70256 | 162.59 | 185.0 |
| 4-Methyloctane | 2216-34-4 | $\mathrm{C}_{9} \mathrm{H}_{20}$ | 128.255 | -113.3 | 142.4 | 1 | 0.7199 | 178.16 | 207.2 |
| $n$-Nonane | 111-84-2 | $\mathrm{C}_{9} \mathrm{H}_{20}$ | 128.255 | -53.46 | 150.82 | 1 | 0.7177 | 178.70 | 207.2 |
| $n$-Decane | 124-18-5 | $\mathrm{C}_{10} \mathrm{H}_{22}$ | 142.282 | -29.6 | 174.15 | 1 | 0.7301 | 194.88 | 229.4 |
| $n$-Undecane | 1120-21-4 | $\mathrm{C}_{11} \mathrm{H}_{24}$ | 156.309 | -25.5 | 195.9 | 1 | 0.7402 | 211.17 | 251.6 |
| $n$-Dodecane | 112-40-3 | $\mathrm{C}_{12} \mathrm{H}_{26}$ | 170.334 | -9.57 | 216.32 | 1 | 0.7487 | 227.51 | 273.8 |
| $n$-Tridecane | 629-50-5 | $\mathrm{C}_{13} \mathrm{H}_{28}$ | 184.361 | -5.4 | 235.47 | 1 | 0.7564 | 243.73 | 296.0 |

TABLE 2.2.1 (Continued)

| Compound | CAS no. | Molecular formula | Molecular weight, MWg/mol | m.p. ${ }^{\circ} \mathrm{C}$ | b.p. ${ }^{\circ} \mathrm{C}$ | Fugacity ratio, F at $25^{\circ} \mathrm{C}^{*}$ | Density, $\rho \mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ | Molar volume, $\mathrm{V}_{\mathrm{M}} \mathrm{cm}^{3} / \mathrm{mol}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  | $\mathrm{MW} / \rho$ at $20^{\circ} \mathrm{C}$ | Le Bas |
| $n$-Tetradecane | 629-59-4 | $\mathrm{C}_{14} \mathrm{H}_{30}$ | 198.388 | 5.82 | 253.58 | 1 | 0.7628 | 260.08 | 318.2 |
| $n$-Pentadecane | 629-62-9 | $\mathrm{C}_{15} \mathrm{H}_{32}$ | 212.415 | 9.95 | 270.6 | 1 | 0.7685 | 276.40 | 340.4 |
| $n$-Hexadecane | 544-76-3 | $\mathrm{C}_{16} \mathrm{H}_{34}$ | 226.441 | 18.12 | 286.86 | 1 | 0.77344 | 292.77 | 362.6 |
| $n$-Heptadecane | 629-78-7 | $\mathrm{C}_{17} \mathrm{H}_{36}$ | 240.468 | 22.0 | 302.0 | 1 | 0.7780 | 309.08 | 384.8 |
| $n$-Octadecane | 593-45-3 | $\mathrm{C}_{18} \mathrm{H}_{38}$ | 254.495 | 28.2 | 316.3 | 0.930 | 0.7819 | 325.48 | 407.0 |
| $n$-Eicosane | 112-95-8 | $\mathrm{C}_{20} \mathrm{H}_{42}$ | 282.547 | 36.6 | 343 | 0.769 | 0.7887 | 358.24 | 451.4 |
| $n$-Tetracosane | 646-31-1 | $\mathrm{C}_{24} \mathrm{H}_{50}$ | 338.654 | 50.4 | 391.3 | 0.563 | 0.7991 | 423.79 | 540.2 |
| $n$-Hexacosane | 630-01-3 | $\mathrm{C}_{26} \mathrm{H}_{54}$ | 366.707 | 56.1 | 412.2 | 0.495 | 0.8032 | 456.56 | 584.6 |
| Cycloalkanes: |  |  |  |  |  |  |  |  |  |
| Cyclopentane | 287-92-3 | $\mathrm{C}_{5} \mathrm{H}_{10}$ | 70.133 | -93.4 | 49.3 | 1 | 0.7454 | 94.09 | 99.5 |
| Methylcyclopentane | 96-37-7 | $\mathrm{C}_{6} \mathrm{H}_{12}$ | 84.159 | -142.42 | 71.8 | 1 | 0.7487 | 112.41 | 121.7 |
| 1,1,3-Trimethylcyclopentane | 4516-69-2 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | -142.4 | 104.9 | 1 | 0.7483 | 149.96 | 166.1 |
| Propylcyclopentane | 2040-96-2 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | -117.3 | 131 | 1 | 0.7763 | 144.55 | 166.1 |
| Pentylcyclopentane | 3741-00-2 | $\mathrm{C}_{10} \mathrm{H}_{20}$ | 140.266 | -83 | 180 | 1 | 0.7912 | 177.28 | 210.5 |
| Cyclohexane | 110-82-7 | $\mathrm{C}_{6} \mathrm{H}_{12}$ | 84.159 | 6.59 | 80.73 | 1 | 0.7786 | 108.09 | 118.2 |
| Methylcyclohexane | 108-87-2 | $\mathrm{C}_{7} \mathrm{H}_{14}$ | 98.186 | -126.6 | 100.93 | 1 | 0.7694 | 127.61 | 140.4 |
| 1,2-cis-Dimethylcyclohexane | 2207-01-4 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | -49.8 | 129.8 | 1 | 0.7963 | 140.92 | 162.6 |
| 1,4-trans-Dimethylcyclohexane | 2207-04-7 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | -36.93 | 119.4 | 1 | 0.7626 | 147.15 | 162.6 |
| 1,1,3-Trimethylcyclohexane | 3073-66-3 | $\mathrm{C}_{9} \mathrm{H}_{18}$ | 126.239 | -65.7 | 136.6 | 1 | 0.7664 | 165.72 | 184.8 |
| Ethylcyclohexane | 1678-91-7 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | -111.3 | 131.9 | 1 | 0.7880 | 142.40 | 162.6 |
| Cycloheptane | 291-64-5 | $\mathrm{C}_{7} \mathrm{H}_{14}$ | 98.186 | -8.46 | 118.4 | 1 | 0.8098 | 121.25 | 136.4 |
| Cyclooctane | 292-64-8 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | 14.59 | 149 | 1 | 0.8340 | 134.55 | 154.1 |
| cis-Decalin | 493-01-6 | $\mathrm{C}_{10} \mathrm{H}_{18}$ | 138.250 | -42.9 | 195.8 | 1 | 0.8931 | 154.80 | 184.6 |
| trans-Decalin | 493-02-7 | $\mathrm{C}_{10} \mathrm{H}_{18}$ | 138.250 | -30.4 | 187.3 | 1 | 0.8662 | 159.60 | 184.6 |
| Alkenes: |  |  |  |  |  |  |  |  |  |
| 2-Methylpropene | 115-11-7 | $\mathrm{C}_{4} \mathrm{H}_{8}$ | 56.107 | -140.7 | -6.9 | 1 | 0.5942 | 94.42 | 88.8 |
| 1-Butene | 106-98-9 | $\mathrm{C}_{4} \mathrm{H}_{8}$ | 56.107 | -185.34 | -6.26 | 1 | 0.5951 | 94.28 | 88.8 |
| 2-Methyl-1-butene | 563-46-2 | $\mathrm{C}_{5} \mathrm{H}_{10}$ | 70.133 | -137.53 | 31.2 | 1 | 0.6504 | 107.83 | 111.0 |
| 3-Methyl-1-butene | 563-45-1 | $\mathrm{C}_{5} \mathrm{H}_{10}$ | 70.133 | -168.43 | 20.1 | 1 | 0.6272 | 111.82 | 111.0 |
| 2-Methyl-2-butene | 513-35-9 | $\mathrm{C}_{5} \mathrm{H}_{10}$ | 70.133 | -133.72 | 38.56 | 1 | 0.6623 | 105.89 | 111.0 |
| 1-Pentene | 109-67-1 | $\mathrm{C}_{5} \mathrm{H}_{10}$ | 70.133 | -165.12 | 29.96 | 1 | 0.6405 | 109.50 | 111.0 |
| cis-2-Pentene | 627-20-3 | $\mathrm{C}_{5} \mathrm{H}_{10}$ | 70.133 | -151.36 | 36.93 | 1 | 0.6556 | 106.98 | 111.0 |
| 2-Methyl-1-pentene | 763-29-1 | $\mathrm{C}_{6} \mathrm{H}_{12}$ | 84.159 | -135.7 | 62.1 | 1 | 0.6799 | 123.78 | 133.2 |
| 4-Methyl-1-pentene | 691-37-2 | $\mathrm{C}_{6} \mathrm{H}_{12}$ | 84.159 | -153.6 | 53.9 | 1 | 0.6642 | 126.71 | 133.2 |


| 1-Hexene | 592-41-6 | $\mathrm{C}_{6} \mathrm{H}_{12}$ | 84.159 | -139.76 | 63.48 | 1 | 0.6732 | 125.01 | 133.2 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1-Heptene | 592-76-7 | $\mathrm{C}_{7} \mathrm{H}_{14}$ | 98.186 | -118.9 | 93.64 | 1 | 0.6970 | 140.87 | 155.4 |
| 1-Octene | 111-66-0 | $\mathrm{C}_{8} \mathrm{H}_{16}$ | 112.213 | -101.7 | 121.29 | 1 | 0.7149 | 156.96 | 177.6 |
| 1-Nonene | 124-11-8 | $\mathrm{C}_{9} \mathrm{H}_{18}$ | 126.239 | -81.3 | 146.9 | 1 | 0.7292 | 173.12 | 199.8 |
| 1-Decene | 872-05-9 | $\mathrm{C}_{10} \mathrm{H}_{20}$ | 140.266 | -66.3 | 170.5 | 1 | 0.7408 | 189.34 | 222.0 |
| Dienes: |  |  |  |  |  |  |  |  |  |
| 1,3-Butadiene | 106-99-0 | $\mathrm{C}_{4} \mathrm{H}_{6}$ | 54.091 | -108.91 | -4.41 | 1 | 0.6211 | 87.09 | 81.4 |
| 2-Methyl-1,3-butadiene (Isoprene) | 78-79-5 | $\mathrm{C}_{5} \mathrm{H}_{8}$ | 68.118 | -145.9 | 34.0 | 1 | 0.6809 | 100.04 | 103.6 |
| 2,3-Dimethyl-1,3-butadiene | 513-81-5 | $\mathrm{C}_{6} \mathrm{H}_{10}$ | 82.143 | -76 | 68.8 | 1 | 0.7267 | 113.04 | 125.8 |
| 1,4-Pentadiene | 591-93-5 | $\mathrm{C}_{5} \mathrm{H}_{8}$ | 68.118 | -148.2 | 26 | 1 | 0.6608 | 103.08 | 103.6 |
| 1,5-Hexadiene | 592-42-7 | $\mathrm{C}_{6} \mathrm{H}_{10}$ | 82.143 | -140.7 | 59.4 | 1 | 0.6923 | 118.65 | 125.8 |
| 1,6-Heptadiene | 3070-53-9 | $\mathrm{C}_{7} \mathrm{H}_{12}$ | 96.170 | -129 | 90 | 1 | 0.714 | 134.69 | 148.0 |
| Alkynes: |  |  |  |  |  |  |  |  |  |
| 1-Butyne | 107-00-6 | $\mathrm{C}_{4} \mathrm{H}_{6}$ | 54.091 | -125.7 | 8.08 | 1 | 0.650 | 83.22 | 81.4 |
| 1-Pentyne | 627-19-0 | $\mathrm{C}_{5} \mathrm{H}_{8}$ | 68.118 | -90 | 40.1 | 1 | 0.6901 | 98.71 | 103.6 |
| 1-Hexyne | 693-02-7 | $\mathrm{C}_{6} \mathrm{H}_{10}$ | 82.143 | -131.9 | 71.3 | 1 | 0.7155 | 114.81 | 125.8 |
| 1-Heptyne | 628-71-7 | $\mathrm{C}_{7} \mathrm{H}_{12}$ | 96.170 | -81 | 99.7 | 1 | 0.7328 | 131.24 | 148.0 |
| 1-Octyne | 629-05-0 | $\mathrm{C}_{8} \mathrm{H}_{14}$ | 110.197 | -79.3 | 126.3 | 1 | 0.7461 | 147.70 | 170.2 |
| 1-Nonyne | 3452-09-3 | $\mathrm{C}_{9} \mathrm{H}_{16}$ | 124.223 | -50 | 150.8 | 1 | 0.7568 | 164.14 | 192.4 |
| Cycloalkenes: |  |  |  |  |  |  |  |  |  |
| Cyclopentene | 142-29-0 | $\mathrm{C}_{5} \mathrm{H}_{8}$ | 68.118 | -135.0 | 44.2 | 1 | 0.772 | 88.24 | 92.1 |
| Cyclohexene | 110-83-8 | $\mathrm{C}_{6} \mathrm{H}_{10}$ | 82.143 | -103.5 | 82.98 | 1 | 0.8110 | 101.29 | 110.8 |
| 1-Methylcyclohexene | 591-49-1 | $\mathrm{C}_{7} \mathrm{H}_{12}$ | 96.170 | -120.4 | 110.3 | 1 | 0.8102 | 118.70 | 133.0 |
| Cycloheptene | 628-92-2 | $\mathrm{C}_{7} \mathrm{H}_{12}$ | 96.170 | -56 | 115 | 1 | 0.8228 | 116.88 | 129.0 |
| cis-Cyclooctene | 931-87-3 | $\mathrm{C}_{8} \mathrm{H}_{14}$ | 110.197 | -12 | 138 | 1 | 0.8472 | 130.07 | 146.7 |
| trans-Cyclooctene | 931-89-5 | $\mathrm{C}_{8} \mathrm{H}_{14}$ | 110.197 | -59 | 143 | 1 | 0.8483 | 129.90 | 146.7 |
| 1,4-Cyclohexadiene | 628-41-1 | $\mathrm{C}_{6} \mathrm{H}_{8}$ | 80.128 | -49.2 | 85.5 | 1 | 0.8471 | 94.59 | 103.4 |
| 1,3,5-Cycloheptatriene | 544-25-2 | $\mathrm{C}_{7} \mathrm{H}_{8}$ | 92.139 | -79.5 | 117 | 1 | 0.8875 | 103.82 | 114.2 |
| $d$-Limonene | 5989-27-5 | $\mathrm{C}_{10} \mathrm{H}_{16}$ | 136.234 | -74.0 | 178 | 1 | 0.8403 | 162.13 | 192.2 |
| $\alpha$-Pinene | 80-56-8 | $\mathrm{C}_{10} \mathrm{H}_{16}$ | 136.234 | -64 | 156.2 | 1 | 0.8582 | 158.74 | 183.7 |
| $\beta$-Pinene | 127-91-3 | $\mathrm{C}_{10} \mathrm{H}_{16}$ | 136.234 | -61.5 | 166 | 1 | 0.8694 | 156.70 | 183.7 |

[^1]TABLE 2.2.2
Summary of selected physical-chemical properties of aliphatic and cyclic hydrocarbons at $25^{\circ} \mathrm{C}$
Selected properties

| Compound | Selected properties |  |  |  |  |  | Henry's law constant $\mathrm{H} /\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)$ calculated P/C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Vapor pressure |  | Solubility |  |  | $\log K_{\text {ow }}$ |  |
|  | Ps/Pa | $\mathrm{P}_{\mathbf{L}} / \mathbf{P a}$ | $\mathrm{S} /\left(\mathrm{g} / \mathrm{m}^{3}\right)$ | $\mathrm{C}^{5} /\left(\mathrm{mol} / \mathrm{m}^{3}\right.$ ) | $\mathrm{C}_{\mathrm{L}} /\left(\mathrm{mol} / \mathrm{m}^{3}\right)$ |  |  |
| Alkanes: |  |  |  |  |  |  |  |
| Isobutane (2-Methylpropane) | 357000 | 357000 | 48.9 | 0.8413 | 0.8413 | 2.76 | 120435* |
| 2,2-Dimethylpropane | 172000 | 172000 | 33.2 | 0.4602 | 0.4602 | 3.11 | 220195* |
| $n$-Butane | 243000 | 243000 | 61.4 | 1.0564 | 1.0564 | 2.90 | 95915* |
| 2-Methylbutane (Isopentane) | 91640 | 91640 | 47.8 | 0.6625 | 0.6625 | 2.30 | 138320 |
| 2,2-Dimethylbutane | 42600 | 42600v | 18.4 | 0.2135 | 0.2135 | 3.82 | 199515 |
| 2,3-Dimethylbutane | 32010 | 32010 | 19.1 | 0.2216 | 0.2216 | 3.85 | 144422 |
| 2,2,3-Trimethylbutane | 13652 | 13652 | 4.38 | 0.0437 | 0.0437 |  | 312320 |
| $n$-Pentane | 68400 | 68400 | 38.5 | 0.5336 | 0.5336 | 3.45 | 128180 |
| 2-Methylpentane (Isohexane) | 28200 | 28200 | 13.8 | 0.1601 | 0.1601 | 2.80 | 176097 |
| 3-Methylpentane | 25300 | 25300 | 12.8 | 0.1485 | 0.1485 | 3.60 | 170330 |
| 2,2-Dimethylpentane | 14000 | 14000 | 4.4 | 0.0439 | 0.0439 | 3.10 | 318825 |
| 2,4-Dimethylpentane | 13100 | 13100 | 4.06 | 0.0405 | 0.0405 | 3.10 | 323312 |
| 3,3-Dimethylpentane | 10940 | 10940 | 5.94 | 0.0593 | 0.0593 |  | 184550 |
| 2,2,4-Trimethylpentane (Isooctane) | 6560 | 6560 | 2.44 | 0.0214 | 0.0214 |  | 307110 |
| 2,3,4-Trimethylpentane | 3600 | 3600 | 2.0 | 0.0119 | 0.0119 |  | 205614 |
| $n$-Hexane | 20200 | 20200 | 9.5 | 0.1102 | 0.1102 | 4.11 | 183235 |
| 2-Methylhexane (Isoheptane) | 8780 | 8780 | 2.54 | 0.0253 | 0.0253 |  | 346370 |
| 3-Methylhexane | 8210 | 8210 | 3.3 | 0.0329 | 0.0329 |  | 249290 |
| 2,2,5-Trimethylhexane | 2210 | 2210 | 1.15 | 0.0090 | 0.0090 | 4.50 | 246472 |
| $n$-Heptane | 6110 | 6110 | 2.93 | 0.0292 | 0.0292 | 5.00 | 208955 |
| 2-Methylheptane | 2600 | 2600 | 0.85 | 0.00744 | 0.0074 |  | 349410 |
| $n$-Octane | 1800 | 1800 | 0.66 | 0.005778 | 0.0058 | 5.15 | 311536 |
| $n$-Nonane | 571 | 571 | 0.22 | 0.001715 | 0.0017 | 5.65 | 332880 |
| $n$-Decane | 175 | 175 | 0.052 | 0.000365 | 0.00037 | 6.25 | 478840 |
| $n$-Undecane | 52.2 | 52.2 | 0.004 | 0.000026 | 0.000026 |  | 2039835 |
| $n$-Dodecane | 18.02 | 18.02 | 0.0037 | 0.000022 | 0.000022 | 6.80 | 829570 |
| $n$-Tridecane | 6.682 | 6.682 |  |  |  |  |  |
| $n$-Tetradecane | 1.804 | 1.804 |  |  |  | 8.00 |  |
| $n$-Hexadecane | 0.191 | 0.191 |  |  |  |  |  |
| $n$-Heptadecane | 0.0615 | 0.0615 |  |  |  |  |  |
| n-Octadecane | 0.02 | 0.019 |  |  |  |  |  |


| $n$-Eicosane | 0.00209 | 0.00161 |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Cycloalkanes: |  |  |  |  |  |  |  |
| Cyclopentane | 42400 | 42400 | 166 | 2.3669 | 2.3669 | 3.00 | 17915 |
| Methylcyclopentane | 18300 | 18300 | 43 | 0.5109 | 0.5109 | 3.37 | 35815 |
| 1,1,3-Trimethylcyclopentane | 5300 | 5300 | 3.73 | 0.0332 | 0.0332 |  | 159440 |
| Propylcyclopentane | 1640 | 1640 | 2.04 | 0.0182 | 0.0182 |  | 90210 |
| Pentylcyclopentane | 152 | 152 | 0.115 | 0.0008 | 0.0008 |  | 185395 |
| Cyclohexane | 13014 | 13014 | 58 | 0.6892 | 0.6892 | 3.44 | 18885 |
| Methylcyclohexane | 6180 | 6180 | 15.1 | 0.1538 | 0.1538 | 3.88 | 40185 |
| 1,2-cis-Dimethylcyclohexane | 1930 | 1930 | 6 | 0.0535 | 0.0535 |  | 36095 |
| 1,4-trans-Dimethylcyclohexane | 3020 | 3020 | 3.84 | 0.0342 | 0.0342 |  | 88250 |
| 1,1,3-Trimethylcyclohexane | 1480 | 1480 | 1.77 | 0.0140 | 0.0140 |  | 105560 |
| Cycloheptane | 2924 | 2924 | 23.5 | 0.2393 | 0.2393 |  | 12220 |
| Cyclooctane | 748 | 748 | 5.80 | 0.0517 | 0.0517 | 4.45 | 14470 |
| Alkenes: |  |  |  |  |  |  |  |
| 2-Methylpropene | 304000 | 304000 | 263 | 4.6875 | 4.6875 |  | 21620* |
| 1-Butene | 297000 | 297000 | 222 | 3.9567 | 3.9567 |  | 25610* |
| 2-Methyl-1-butene | 81330 | 81330 |  |  |  |  |  |
| 3-Methyl-1-butene | 120000 | 120000 | 130 | 1.8536 | 1.8536 |  | 54670* |
| 2-Methyl-2-butene | 62410 | 62410 | 325 | 4.634 | 4.634 |  | 13470 |
| 1-Pentene | 85000 | 85000 | 148 | 2.1103 | 2.1103 | 2.20 | 40280 |
| cis-2-Pentene | 66000 | 66000 |  |  |  | 2.20 |  |
| 2-Methyl-1-pentene | 26000 | 26000 | 78 | 0.9268 | 0.9268 |  | 28050 |
| 4-Methyl-1-pentene | 36100 | 36100 | 48 | 0.5703 | 0.5703 | 2.50 | 63295 |
| 1-Hexene | 24800 | 24800 | 50 | 0.5941 | 0.5941 | 3.39 | 41743 |
| 1-Heptene | 7510 | 7510 | 18.3 | 0.1864 | 0.1864 | 3.99 | 40295 |
| 1-Octene | 2320 | 2320 | 2.7 | 0.0241 | 0.0241 | 4.57 | 96420 |
| 1-Nonene | 712 | 712 | 1.12 | 0.0089 | 0.0089 | 5.15 | 80250 |
| 1-Decene | 218 | 218 |  |  |  |  |  |
| Dienes: |  |  |  |  |  |  |  |
| 1,3-Butadiene | 281000 | 281000 | 735 | 13.588 | 13.588 | 1.99 | 7458* |
| 2-Methyl-1,3-butadiene (Isoprene) | 73300 | 73300 | 642 | 9.4248 | 9.4248 |  | 7780 |
| 2,3-Dimethyl-1,3-butadiene | 20160 | 20160 | 327 | 3.9809 | 3.9809 |  | 5065 |
| 1,4-Pentadiene | 98000 | 98000 | 558 | 8.1917 | 8.1917 | 2.48 | 11965 |
| 1,5-Hexadiene | 29690 | 29690 | 169 | 2.0574 | 2.0574 | 2.75 | 14430 |
| 1,6-Heptadiene |  |  | 44 | 0.4575 | 0.4575 |  |  |

(Continued)

TABLE 2.2.2 (Continued)

| Compound | Selected properties |  |  |  |  |  | Henry's law constant $\mathrm{H} /\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)$ calculated P/C |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Vapor pressure |  | Solubility |  |  | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {ow }}$ |  |
|  | Ps/Pa | $\mathrm{P}_{\mathbf{L}} / \mathbf{P a}$ | $\mathrm{S} /\left(\mathrm{g} / \mathrm{m}^{3}\right)$ | $\mathrm{C}^{5} /\left(\mathrm{mol} / \mathrm{m}^{3}\right)$ | $\mathrm{C}_{\mathrm{L}} /\left(\mathrm{mol} / \mathrm{m}^{3}\right)$ |  |  |
| Alkynes: |  |  |  |  |  |  |  |
| 1-Butyne | 188000 | 188000 | 2870 | 53.059 | 53.059 |  | 1910* |
| 1-Pentyne | 57600 | 57600 | 1570 | 23.048 | 23.048 | 1.98 | 2500 |
| 1-Hexyne | 18140 | 18140 | 360 | 4.3830 | 4.3830 | 2.73 | 4140 |
| 1-Heptyne | 7500 | 7000 | 94 | 0.9774 | 0.9774 | 2.98 | 7675 |
| 1-Octyne | 1715 | 1715 | 24 | 0.2178 | 0.2178 |  | 7875 |
| 1-Nonyne |  |  | 7.2 | 0.0580 | 0.0580 |  |  |
| Cycloalkenes: |  |  |  |  |  |  |  |
| Cyclopentene | 50710 | 50706 | 535 | 7.8540 | 7.8540 | 2.48 | 6455 |
| Cyclohexene | 11850 | 11850 | 213 | 2.5928 | 2.5928 | 2.86 | 4570 |
| 1-Methylcyclohexene | 4689 | 4689 | 52 | 0.5407 | 0.5407 |  | 8670 |
| Cycloheptene | 2670 | 2670 | 66 | 0.6863 | 0.6863 |  | 3890 |
| Cyclooctene | 1010 | 1010 | 22.9 | 0.2078 | 0.2078 | 2.47 | 4860 |
| 1,4-Cyclohexadiene | 9009 | 9009 | 800 | 9.9840 | 9.9840 |  | 902 |
| 1,3,5-Cycloheptatriene | 3140 | 3140 | 620 | 7.7376 | 7.7376 | 2.63 | 467 |
| $d$-Limonene | 270 | 270 | 13.8 | 0.1013 | 0.1013 |  | 2665 |
| $\alpha$-Pinene | 582 | 582 |  |  |  |  |  |
| $\beta$-Pinene | 395 | 395 |  |  |  |  |  |

* Vapor pressure exceeds atmospheric pressure, Henry's law constant $\mathrm{H} /\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)=101325 \mathrm{~Pa} / \mathrm{C}^{\mathrm{s}} \mathrm{mol} / \mathrm{m}^{3}$.

TABLE 2.2.3
Suggested half-life classes of hydrocarbons in various environmental compartments at $25^{\circ} \mathrm{C}$

| Compound | $\begin{aligned} & \text { Air } \\ & \text { class } \end{aligned}$ | Water class | Soil <br> class | Sediment class |
| :---: | :---: | :---: | :---: | :---: |
| Alkanes: |  |  |  |  |
| $n$-Pentane | 2 | 5 | 6 | 7 |
| $n$-Hexane | 2 | 5 | 6 | 7 |
| $n$-Octane | 2 | 5 | 6 | 7 |
| $n$-Decane | 2 | 5 | 6 | 7 |
| $n$-Dodecane | 2 | 5 | 6 | 7 |
| Cycloalkanes: |  |  |  |  |
| Cyclopentane | 2 | 5 | 5 | 6 |
| Methylcyclopentane | 2 | 5 | 5 | 6 |
| Cyclohexane | 2 | 5 | 5 | 6 |
| Methylcyclohexane | 2 | 5 | 5 | 6 |
| Cyclooctane | 2 | 5 | 5 | 6 |
| Alkenes: |  |  |  |  |
| 1-Pentene | 1 | 4 | 5 | 6 |
| 1-Octene | 1 | 4 | 5 | 6 |
| 1,3-Butadiene | 1 | 4 | 5 | 6 |
| 1,4-Pentadiene | 1 | 4 | 5 | 6 |
| Alkynes: |  |  |  |  |
| 1-Hexyne | 1 | 4 | 5 | 6 |
| Cycloalkenes: |  |  |  |  |
| Cyclopentene | 1 | 4 | 5 | 6 |
| Cyclohexene | 1 | 4 | 5 | 6 |

where,

| Class | Mean half-life (hours) | Range (hours) |
| :--- | :--- | :--- |
| 1 | 5 | $<10$ |
| 2 | $17(\sim 1$ day $)$ | $10-30$ |
| 3 | $55(\sim 2$ days $)$ | $30-100$ |
| 4 | $170(\sim 1$ week $)$ | $100-300$ |
| 5 | $550(\sim 3$ weeks $)$ | $300-1,000$ |
| 6 | $1700(\sim 2$ months $)$ | $1,000-3,000$ |
| 7 | $5500(\sim 8$ months $)$ | $3,000-10,000$ |
| 8 | $17000(\sim 2$ years $)$ | $10,000-30,000$ |
| 9 | $55000(\sim 6$ years $)$ | $>30,000$ |



FIGURE 2.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alkanes.


FIGURE 2.2.2 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.


FIGURE 2.2.3 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alkanes.


FIGURE 2.2.4 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.


FIGURE 2.2.5 Octanol-water partition coefficient versus Le Bas molar volume for alkanes.


FIGURE 2.2.6 Octanol-water partition coefficient versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.


FIGURE 2.2.7 Henry's law constant versus Le Bas molar volume for alkanes.


FIGURE 2.2.8 Henry's law constant versus Le Bas molar volume for aliphatic and cyclic hydrocarbons.


FIGURE 2.2.9 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alkanes.


FIGURE 2.2.10 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aliphatic and cyclic hydrocarbons.

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## 3 Mononuclear Aromatic Hydrocarbons

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### 3.1 LIST OF CHEMICALS AND DATA COMPILATIONS

### 3.1.1 Mononuclear aromatic hydrocarbons

### 3.1.1.1 Benzene



Common Name: Benzene
Synonym: benzol, cyclohexatriene
Chemical Name: benzene
CAS Registry No: 71-43-2
Molecular Formula: $\mathrm{C}_{6} \mathrm{H}_{6}$
Molecular Weight: 78.112
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
5.49 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
80.09 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8765 (Weast 1982-1983)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$89.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
96.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $33.843,30.726\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)
Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.916 (Tsonopoulos \& Prausnitz 1971)
9.866 (Riddick et al. 1986)
9.87 (exptl., Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
35.564 (Tsonopoulos \& Prausnitz 1971)
35.4, 44.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$1850 \quad\left(30^{\circ} \mathrm{C}\right.$, shake flask-interferometer, Gross \& Saylor 1931)
1786 (shake flask-turbidimetric method, Stearns et al. 1947)
1402 (residue-volume method, Booth \& Everson 1948)
1740 (shake flask-UV spec., Andrews \& Keefer 1949)
1860 (shake flask-UV, Klevens 1950)
1790* (shake flask-UV, Bohon \& Claussen 1951)
1755 (shake flask-UV, McDevit \& Long 1952)
1718 (shake flask-UV, Morrison \& Billett 1952)
1796 (Hayashi \& Sasaki 1956; quoted, Keeley et al. 1988)
1780, 1823 (selected, calculated-molar volume, Lindenburg 1956; quoted, Horvath 1982)
1760 (Brady \& Huff 1958)
1740* (shake flask-UV, measured range $0.4-45^{\circ} \mathrm{C}$, Arnold et al. 1958)
$\mathrm{S} /(\mathrm{wt} . \%)=0.1806-0.001095 \cdot\left(\mathrm{t}^{\circ} \mathrm{C}\right)+3.170 \times 10^{-5} \cdot\left(\mathrm{t}^{\circ} \mathrm{C}\right)^{2}$; temp range $5-45^{\circ} \mathrm{C}$ (shake flask-UV, Arnold et al. 1958); or $\mathrm{S} /(\mathrm{wt} . \%)=0.1784-0.0007436 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+1.1906 \times 10^{-5} \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+1.217 \times 10^{-7} \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $5-45^{\circ} \mathrm{C}$ (shake flask-UV, Arnold et al. 1958)
$1800^{*} \quad\left(24^{\circ} \mathrm{C}\right.$, shake flask-UV, measured range $0.8-64.5^{\circ} \mathrm{C}$, Alexander 1959)
$1890 \quad\left(35^{\circ} \mathrm{C}\right.$, shake flask-UV spectrophotometry, Hine et al. 1962)
1742* (shake flask-UV, measured range $17-63^{\circ} \mathrm{C}$, Franks et al. 1963)

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1780
    (shake flask-GC, McAuliffe 1963, 1966)
2100*
    (20}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , polythermic method, measured range 20-79.5}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , Udovenko & Aleksandrova 1963)
1778
    (calculated-group contribution, Irmann 1965; quoted, Horvath 1982)
2167
    (vapor saturation-UV, Worley 1967)
1740
    (21 }\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , extraction by nonpolar resins/elution, Chey & Calder 1972)
1765* (shake flask-GC, measured range 4-25*}\textrm{C}\mathrm{ (, Leinonen 1972)
1830* (shake flask-UV spectroscopy, measured range 25-55*}\textrm{C}\mathrm{ , Bradley et al. 1973)
1755 (shake flask-GC, Polak & Lu 1973)
1755* (shake flask-GC, measured range 25-84.7}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , Price 1973)
1765 (shake flask-GC, Leinonen & Mackay 1973)
1760* (shake flask-UV, measured range 4.5-20.1 }\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , Brown & Wasik 1974)
1906 (shake flask-UV, Vesala 1974)
1769 (shake flask-GC, Mackay et al. 1975)
1780 (shake flask-GC, Mackay & Shiu 1975)
1740 (shake flask-GC, Price 1976)
1791* (generator column-HPLC/UV, May et al. 1978; May 1980)
S}/(\mu\textrm{g}/\textrm{kg})=[1833+0.3166\cdot(\textrm{t}/\mp@subsup{}{}{\circ}\textrm{C}\mp@subsup{)}{}{2}-0.6838\cdot(\textrm{t}/\mp@subsup{}{}{\circ}\textrm{C}\mp@subsup{)}{}{3}]\times1\mp@subsup{0}{}{3};\mathrm{ ; temp range 0.2-25.8}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ (generator column-HPLC/UV,
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May et al. 1978, 1980)
$\log x=424.544 /(\mathrm{T} / \mathrm{K})^{2}-2955.82 /(\mathrm{T} / \mathrm{K})+1.6606$; temp range $0-55^{\circ} \mathrm{C}$ (Ueda et al. 1978)
1769 (shake flask-fluorescence spectrophotometry, Aquan-Yuen et al. 1979)
1734* $\quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Ben-Naim \& Wilf 1979)
$1790^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, Bittrich et al. 1979)
1820-1930 (elution chromatography-UV, Schwarz 1980)
1750 (shake flask-LSC, Banerjee et al. 1980)
1610* (vapor saturation-UV spec., measured range 5-45 ${ }^{\circ}$ C, Sanemasa et al. 1981)
1787 (shake flask-GC, Chiou et al. 1982; 1983)
1620* (vapor saturation-UV spec., measured range $5-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
1792* (generator column-HPLC/UV, May et al. 1983)
1789 (generator column-HPLC, Wasik et al. 1983)
1809 (HPLC- $\mathrm{k}^{\prime}$ correlation, converted from reported $\gamma_{\mathrm{W}}$, Hafkenscheid \& Tomlinson 1983a)
1617 (vapor saturation-UV spec., Sanemasa et al. 1984)
1810 (shake flask-radiometric method, Lo et al. 1986)
1695 (shake flask-GC, Keeley et al. 1988)
1650 (shake flask-GC, Coutant \& Keigley 1988)
1770* (IUPAC recommended, temp range $0-70^{\circ} \mathrm{C}$, Shaw 1989a)
$\mathrm{S} /(\mathrm{g} / 100 \mathrm{~g}$ soln $)=5.5773-4.6067 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.2504 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})^{2}-1.0489 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{3} ;$ temp range $0-70^{\circ} \mathrm{C}$
(summary of literature data, Shaw 1989a)
1732* $\quad\left(20^{\circ} \mathrm{C}\right.$, activity coefficient-GC, Cooling et al. 1992)
$1840^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, equilibrium flow cell-GC, measured range $30-100^{\circ} \mathrm{C}$, Chen \& Wagner 1994a)
$\ln (1 / x)=-6.191+14.03 \cdot[(\mathrm{~T} / \mathrm{K}) / 562.2]^{-1}-3.511 \cdot[(\mathrm{~T} / \mathrm{K}) / 562.2]^{-2}$; temp range $303.15-373.15 \mathrm{~K}$ (equilibrium flow
cell-GC, Chen \& Wagner 1994a)
$\ln x=6.191-14.03 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-1}+3.511 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-2}, \mathrm{~T}_{\mathrm{r}}=\mathrm{T} / \mathrm{T}_{\mathrm{c}}$, the reduced temp, system temp T divided by critical
temp $\mathrm{T}_{\mathrm{c}}$ (Chen \& Wagner 1994c)
1760 (dialysis tubing equilibration-GC. Etzweiler et al. 1995)
$\ln x=-15.544647-1442.4276 /(\mathrm{T} / \mathrm{K})-3.283 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2}$, temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data,
Shiu \& Ma 2000)
$\ln x=-180.368+7524.83 /(\mathrm{T} / \mathrm{K})+25.8585 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calo-
rimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$\begin{array}{ll}12654 & (\mathrm{Hg} \text { manometer, Hovorka \& Dreisbach } 1934) \\ 9960^{*} & \left(20^{\circ} \mathrm{C} \text {, manometer, measured range } 0-50^{\circ} \mathrm{C}, \text { Stuckey \& Saylor 1940) }\right.\end{array}$
$\log (\mathrm{P} / \mathrm{mmHg})=7.12491-1323.06 /(\mathrm{T} / \mathrm{K}-41.23)$; temp range $0-75^{\circ} \mathrm{C}$ (manometer, Stuckey \& Saylor 1940)

11700* $\quad\left(23.7^{\circ} \mathrm{C}\right.$, ebulliometry-manometer, measured range $14.5-80.9^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.89324-1203.835 /\left(219.924+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $14.5-80.9^{\circ} \mathrm{C}$ (ebulliometry-manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
13332* ( $26.1^{\circ} \mathrm{C}$, summary of literature data, Stull 1947)
$11720^{*} \quad\left(23.27^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $10.9-80.9^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91210-1214.645 /\left(221.205+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10.9-80.9^{\circ} \mathrm{C}$ (ebulliometry-manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
12690 (interpolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90565-1211.033 /\left(220.79+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-160^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$23450^{*} \quad\left(39.093^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $7.565-260^{\circ} \mathrm{C}$, Bond \& Thodos 1960$)$
$545800^{*} \quad\left(146.85^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $146.85-286.85^{\circ} \mathrm{C}$, Ambrose et al. 1967)
$32045^{*} \quad\left(46.85^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $46.85-286.85^{\circ} \mathrm{C}$, Ambrose et al.1970)
12700* (extrapolated-Antoine eq., Zwolinski \& Wilhoit, 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90565-1211.033 /\left(220.790+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -11.6 to $103.92^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
12680 (extrapolated, Antoine eq., Boublik et al. 1973; 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10254.2 /(\mathrm{T} / \mathrm{K})]+9.5560$; temp range -58 to $-30^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8146.5 /(\mathrm{T} / \mathrm{K})]+7.833714$; temp range -36.7 to $290.3^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
12339* (24.396 ${ }^{\circ} \mathrm{C}$, ebulliometry, measured range $19.071-32.467^{\circ} \mathrm{C}$, Osborn \& Scott 1978)
19933* ( $32.182^{\circ} \mathrm{C}$, ebulliometry, measured range $32.182-115.697^{\circ} \mathrm{C}$, Scott \& Osborn 1979)
12640* (average, ebulliometry-bubble cap boilers, measured range 290-378 K, Ambrose 1981)
12100 (gas saturation-GC, Politzki et al. 1982)
$\log (\mathrm{P} / \mathrm{atm})=(1-353.214 / \mathrm{T}) \times 10^{\wedge}\left(0.832632-6.72598 \times 10^{4} \cdot \mathrm{~T}+6.38324 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range $280.0-562.6 \mathrm{~K}$ (Cox vapor pressure eq., Chao et al. 1983)
12690, 12680 (interpolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.01905-1204.637 /\left(220.069+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $21.2-105^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Ambrose 1981, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.01788-1203.677 /\left(219.904+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $14.5-80.9^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl.
data of Willingham et al. 1945, Boublik et al. 1984)
12690 (extrapolated, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=9.1064-1885.9 /\left(244.2+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -12 to $3^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90565-1211.033 /\left(220.79+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $8-103^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
12716 (headspace-GC, Hussam \& Carr 1985)
$\log (\mathrm{P} / \mathrm{kPa})=6.02232-1206.33 /\left(220.91+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
12700 (interpolated-Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.0091-2836 /(25.31+\mathrm{T} / \mathrm{K})$; temp range $223-279 \mathrm{~K}$ (solid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=8.45261-1986.69 /(-23.089 \mathrm{C}+\mathrm{T} / \mathrm{K})$; temp range $218-279 \mathrm{~K}$ (solid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.01907-1204.682 /(-53,072+\mathrm{T} / \mathrm{K})$; temp range $279-377 \mathrm{~K}$ (liquid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.06832-1236.034 /(-48.99+\mathrm{T} / \mathrm{K})$; temp range $353-422 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.3607-1466.083 /(-15.44+\mathrm{T} / \mathrm{K})$; temp range $420-502 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.51922-2809.514 /(171.489+\mathrm{T} / \mathrm{K})$; temp range $501-562 \mathrm{~K}$ (Antoine eq.-VI, Stephenson \& Malanowski 1987)
13100* (gas saturation, measured range -15.4 to $40^{\circ} \mathrm{C}$, Liu \& Dickhut 1994)
$\log (\mathrm{P} / \mathrm{mmHg})=31.7718-2.7254 \times 10^{3} /(\mathrm{T} / \mathrm{K})-8.4442 \cdot \log (\mathrm{~T} / \mathrm{K})-5.3534 \times 10^{-9} \cdot(\mathrm{~T} / \mathrm{K})+2.7187 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $279-562 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$\log (\mathrm{P} / \mathrm{kPa})=6.02994-1211.033 /[(\mathrm{T} / \mathrm{K})-52.36]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$653 \quad\left(30^{\circ} \mathrm{C}\right.$, concn ratio-UV, Saylor et al. 1938)
576 (Taha et al. 1966)
442* $\quad\left(20.06^{\circ} \mathrm{C}\right.$, headspace-GC, Brown \& Wasik 1974)
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=21.26071-4445.58 /(\mathrm{T} / \mathrm{K})$; temp range $4.5-20^{\circ} \mathrm{C}$ (regression eq. of exptl. data of Brown \& Wasik 1974, Shiu \& Ma 2000)
555, 530 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}$, calculated-bond contribution, Hine \& Mookerjee 1975)
551 (headspace-GC, Vitenberg et al. 1975)
562, 556 (batch air stripping-GC, calculated-P/C, Mackay et al. 1979)
552* (shake flask-concn. ratio-UV, measured range $10-30^{\circ} \mathrm{C}$, Green \& Frank 1979)
$\log (\mathrm{H} / \mathrm{atm})=8.58-1852.308 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (shake flask-concn-UV, Green \& Frank 1979)
$\ln (\mathrm{H} / \mathrm{atm})=8.58-1852.038 /(\mathrm{T} / \mathrm{K})($ Kavanaugh \& Trussell 1980)
554* (equilibrium cell-concentration ratio-GC/FID, Leighton \& Calo 1981)
$\ln \left(k_{\mathrm{H}} / \mathrm{atm}\right)=19.02-3964 /(\mathrm{T} / \mathrm{K})$; temp range $1.0-27.2^{\circ} \mathrm{C}$ (equilibrium cell-concn ratio, Leighton \& Calo 1981)
610* (vapor-liquid equilibrium-GC, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1981)
608* (vapor-liquid equilibrium-GC, measured range $5-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
562 (gas stripping-GC, Warner et al. 1987)
740; $441 \quad\left(20^{\circ} \mathrm{C}\right.$, EPICS-GC, calculated-P/C, Yurteri et al. 1987)
535; 588; 557; 554; 555 (EPICS-GC/FID; batch air stripping-GC; calculated P/C; direct concentration ratio; calculated-UNIFAC, Ashworth et al. 1988)
$535^{*} \quad$ (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)\right]=5.534-3194 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
586 (concentration ratio, Keeley et al. 1988)
555 (infinite activity coeff. $\gamma^{\infty}$ from solubility measurement, Abraham et al. 1990)
564 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
570* (extrapolated from equilibrium headspace-GC data, measured range $40-80^{\circ} \mathrm{C}$, Ettre et al. 1993)
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=-2.1678537+836.2228 /(\mathrm{T} / \mathrm{K})$; temp range: $45-80^{\circ} \mathrm{C}$ (equilibrium headspace-GC measurements, Ettre et al. 1993)
569 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
604* (equilibrium headspace-GC, measured range $10-30^{\circ} \mathrm{C}$, Perlinger et al. 1993)
535* (static headspace-GC, measured range $25-50^{\circ} \mathrm{C}$, Robbins et al. 1993)
644 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
$488 \quad\left(23^{\circ} \mathrm{C}\right.$, gas stripping-IR, Nielsen et al. 1994)
481* (EPICS-GC/FID, measured range $2-25^{\circ} \mathrm{C}$, Dewulf et al. 1995)
267, $612\left(6.0,25^{\circ} \mathrm{C}\right.$, EPICS-GC/FID, natural seawater with salinity of $35 \%$, Dewulf et al. 1995)
$\ln \mathrm{K}_{\mathrm{AW}}=-3640 /(\mathrm{T} / \mathrm{K})+0.00786 \cdot \mathrm{Z}+10.577$; with Z salinity $0-35.5 \%$, temp range: $2-35^{\circ} \mathrm{C}(\mathrm{EPICS}-\mathrm{GC} / \mathrm{FID}$, Dewulf et al. 1995)
552* (25.4 ${ }^{\circ} \mathrm{C}$, gas stripping-HPLC/UV/fluorescence, Alaee et al. 1996)
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}\right)\right]=21.87689-4672.28 /(\mathrm{T} / \mathrm{K})$; temp range: $4-34.9^{\circ} \mathrm{C}$ and enthalpy of volatilization $\Delta \mathrm{H}_{\mathrm{vol}}=$ $32.2 \mathrm{~kJ} / \mathrm{mol}$ at $20^{\circ} \mathrm{C}$; (gas stripping-HPLC/UV measurements, Alaee et al. 1996)
$485 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
640* (vapor-liquid equilibrium-GC, measured range $10-35^{\circ} \mathrm{C}$, Turner et al. 1996)
$\mathrm{K}_{\mathrm{AW}}=0.0763+0.00211 \cdot(\mathrm{~T} / \mathrm{K})+0.000162 \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $0-50^{\circ} \mathrm{C}$ (vapor-liquid equilibrium-GC measurements with additional lit. data, Turner et al. 1996)
538* (headspace equilibrium-GC, Peng \& Wan 1997)
$\ln \mathrm{K}_{\mathrm{AW}}=7.15-1397 /(\mathrm{T} / \mathrm{K})$; temp range $15-45^{\circ} \mathrm{C}$ (headspace equilibrium-GC, Peng \& Wan 1997)
272 (gas stripping-GC, Altschuh et al. 1999)
$439 \quad\left(20^{\circ} \mathrm{C}\right.$, headspace equilibrium-GC, Peng \& Wan 1998)
$\ln \mathrm{K}_{\mathrm{AW}}=7.44-1448 /(\mathrm{T} / \mathrm{K})$; temp range $0-45^{\circ} \mathrm{C}$ (seawater with salinity of $36 \%$, headspace-GC, Peng \& Wan 1998)
$466 \quad\left(21^{\circ} \mathrm{C}\right.$, headspace equilibrium-GC, de Wolf \& Lieder 1998)
558 (exponential saturator EXPSAT technique, Dohnal \& Hovorka 1999)
580.6 (modified EPICS method-GC, Ryu \& Park 1999)

556 (EPICS-static headspace method-GC/FID, Miller \& Stuart 2000)
$466 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=5.053-1693 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
538* (solid-phase microextraction-GC, measured range $15-40^{\circ} \mathrm{C}$, Bierwagen \& Keller 2001)
$\ln \mathrm{K}_{\mathrm{AW}}=8.1648-2889.4 /(\mathrm{T} / \mathrm{K})$; temp range $15-40^{\circ} \mathrm{C}$ (SPME-GC, Bierwagen \& Keller 2001)
573.4* (EPICS-SPME, measured range $2-60^{\circ} \mathrm{C}$, Görgényi et al. 2002)
$\ln \mathrm{K}_{\mathrm{AW}}=10.01-3430.4 /(\mathrm{T} / \mathrm{K})$; temp range $2-60^{\circ} \mathrm{C}$ (EPICS-SPME method, Görgényi et al. 2002)
514-606 $\quad\left(27^{\circ} \mathrm{C}\right.$, headspace equilibrium-GC, at different solute concn: $0.48-19.1 \mathrm{mg} / \mathrm{L}$, measured temp range 300-315 K, Cheng et al. 2003)
558* (headspace-GC, measured range $10-25^{\circ} \mathrm{C}$, Bakierowska \& Trzeszczyński 2003) $\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=11.663-3920 /(\mathrm{T} / \mathrm{K})$; temp range $10-25^{\circ} \mathrm{C}$, headspace-GC, Bakierowska \& Trzeszczyński 2003)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.13 (shake flask-UV, Fujita et al. 1964)
1.56, 1.65 (shake flask-UV, calculated-M.O. indices, Rogers \& Cammarata 1969)
2.13 (calculated-fragment const., Rekker 1977)
2.13, 1.56, 2.15, 2.03, 2.04 (Hansch \& Leo 1979)
2.39 (HPLC-RT correlation, Veith et al. 1979a)
2.12 (shake flask-LSC, Banerjee et al. 1980)
2.28 (HPLC-k' correlation, Hanai et al. 1981)
2.11 (HPLC-RT correlation, McDuffie 1981)
2.43 (HPLC-k' correlation, McDuffie 1981)
2.16 (HPLC- $\mathrm{k}^{\prime}$ correlation, D'Amboise \& Hanai 1982)
2.13 (shake flask-GC, Watarai et al. 1982)
2.20 (shake flask-HPLC, Hammers et al. 1982)
2.18 (HPLC-k' correlation, Miyake \& Terada 1982)
2.02 (shake flask method, Eadsforth \& Moser 1983)
2.38 (HPLC method, Eadsforth \& Moser 1983)
2.10 (shake flask-GC, Platford 1983)
2.48 (HPLC-RT correlation, Swann et al. 1983)
2.10 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983b)
2.04 (HPLC-RV correlation, Garst 1984)
2.25 (RP-HPLC- $k^{\prime}$ correlation, Rapaport \& Eisenreich 1984)
2.13 (generator column-GC/ECD, Miller et al. 1984)
2.26 (HPLC-k' correlation, De Kock \& Lord 1987)
2.01 (generator column-reversed phase-LC, Schantz \& Martire 1987)
2.16 (RP-HPLC-capacity factor correlation, Sherblom \& Eganhouse 1988)
1.91 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
2.13 (recommended, Sangster 1989, 1993)
2.186 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
2.21 (normal phase-HPLC-k' correlation, Govers \& Evers 1992)
2.13 (recommended, Hansch et al. 1995)
1.97* $\quad\left(24.8^{\circ} \mathrm{C}\right.$, EPICS-GC, measured range $2.2-24.8^{\circ} \mathrm{C}$, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section:
$2.90^{*} \quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range $20.290-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997)
2.80 (head-space GC-FID both phases, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
0.64 (pacific herring, Korn et al. 1977)
0.54 (eels, Ogata \& Miyake 1978; Ogata et al. 1984)
1.10 (fathead minnow, Veith et al. 1980)
1.48, $1.0 \quad$ (algae, fish, Freitag et al. 1984)
1.48 (algae, Geyer et al. 1984)
0.63 (gold fish, Ogata et al. 1984)
$<1.0,3.23$ (fish, activated sludge, Freitag et al. 1985)
0.54, 0.64, 0.63; 1.38 (selected: eels, pacific herring, gold fish; calculated, Howard 1990)
1.63 (S. capricornutum, Herman et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
1.92 (sediment, sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
1.63; 1.82 (Hastings soil pH 5.6; Overton soil pH 7.8, batch equilibrium, Rogers et al. 1980)
1.78 (average of 17 sediments and soils, sorption isotherms by batch equilibrium, Karickhoff 1981)
1.58; 1.73; 1.64 (forest soil pH 5.6 ; forest soil pH 4.2 ; agricultural soil pH 7.4 , Seip et al. 1986)
1.42 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
1.34 (untreated Marlette soil A horizon, organic carbon OC $2.59 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.08, 2.04 (organic cations treated Marlette soil A horizon: HDTMA treated OC 6.48\%; DDTMA treated, OC $4.37 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.65, 2.59, 2.25 (organic cations treated Marlette soil $\mathrm{B}_{\mathrm{t}}$ horizon: HDTMA treated OC $3.72 \%$, DDTMA treated OC $1.98 \%$, NTMA treated, OC $1.18 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.69, 2.66 (organic cations HDTMA treated soils: St. Clair soil $B_{t}$ horizon OC 3.25\%; Oshtemo soil $B_{t}$ horizon OC $0.83 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.89 (aquifer material with $\mathrm{f}_{\mathrm{OC}}$ of 0.006 and measured partition coeff. $\mathrm{K}_{\mathrm{P}}=0.47 \mathrm{~mL} / \mathrm{g}$., Abdul et al. 1990)
1.58, 1.49 (Riddles soil top layer, pH 5.0 ; below top layer pH 5.3 , batch equilibrium, Boyd et al. 1990)
1.82, 1.87 (RP-HPLC-k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
1.74; 1.81 (Captina silt loam pH 4.97 ; McLaurin sandy loam pH 4.43 , batch equilibrium, Walton et al. 1992)
1.75 (average of 5 soils, sorption isotherms by batch equilibrium method-GC, Xing et al. 1994)
1.96 (soil, calculated-molecular connectivity indices, Sabljic et al. 1995)
1.57, 1.62, 1.74 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al. 1995)
1.82, 1.84 (RP-HPLC- $\mathrm{k}^{\prime}$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
$1.84,1.86,1.87,1.88,1.90,1.87,1.90\left(2.3,3.8,6.2,8.0,13.5,18.6,25^{\circ} \mathrm{C}\right.$, natural sediment from River Leie, organic carbon $f_{\text {OC }}=4.12 \%$, EPICS-GC/FID, Dewulf et al. 1999)
2.76, 2.41 (natural zeolite modified with a cation surfactant HDTMA with surface coverage of 100,200 $\mathrm{mmol} / \mathrm{kg}$ at pH 7 , batch equilibrium-sorption isotherm, Li et al. 2000)
1.64, 1.58, 1.78 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%, \mathrm{OC} \geq 0.5 \%, 0.1 \leq \mathrm{OC}<0.5 \%$, average, Delle Site 2001)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{Oм}}$ :
1.26 (Woodburn silt loam soil, $1.9 \%$ organic matter, equilibrium isotherm-GC, Chiou et al. 1983)
1.04 (untreated Marlette soil A horizon, organic matter OM 5.18\%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.89, 1.81 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03\%; DDTMA treated, OM $5.18 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.53, 2.46, 2.08 (organic cations treated Marlette soil $B_{t}$ horizon: HDTMA treated OM 4.85\%, DDTMA treated OM $2.73 \%$, NTMA treated, OM $1.74 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
$2.56,2.53$ (organic cations HDTMA treated soils: St. Clair soil $B_{t}$ horizon OM 4.38\%; Oshtemo soil $B_{t}$ horizon OM $1.12 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.34; 1.14 (high-organic-content soils: Florida peat $-57.1 \%$ C; Michigan muck $-53.7 \%$ C, equilibrium iso-therm-GC, Rutherford \& Chiou 1992)

Environmental Fate Rate Constants, k , or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $\mathrm{t}_{1 / 2}=4.81 \mathrm{~h}$ from water depth of 1 m (calculated, Mackay \& Leinonen 1975; Haque et al. 1980); $\mathrm{k}=0.03 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=23 \mathrm{~d}$ in spring at $8-16^{\circ} \mathrm{C}, \mathrm{k}=0.22 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=31 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{k}=$ $0.054 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ during the periods when volatilization appears to dominate, and $\mathrm{k}=0.101 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=6.9 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in September 9-15, 1980 in marine mesocosm experiments (Wakeham et al. 1983);
$t_{1 / 2} \sim 27 \mathrm{~h}$ from a river of 1 m depth with wind speed $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{s}$ is 2.7 h at $20^{\circ} \mathrm{C}$ (Lyman et al. 1982).

Photolysis: atmospheric photolysis $\mathrm{t}_{1 / 2}=2808-16152 \mathrm{~h}$, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991);
aqueous photolysis $t_{1 / 2}=2808-16152 \mathrm{~h}$, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991);
reaction rate constants, $\mathrm{k}=8.64 \times 10^{-4} \mathrm{~h}^{-1}$ in air, and $\mathrm{k}=1.8 \times 10^{-4} \mathrm{~h}^{-1}$ in water (Mackay et al. 1985).
Oxidation: rate constant k ; and gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated $*$, see reference:
$\mathrm{k}_{\mathrm{OH}}=1.24 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=0.24 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}} \leq 2.3 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2} \geq 5.1 \mathrm{~h} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(0.144 \pm 0.2) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=0.85 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$, with $\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}} *=(1.20 \pm 0.15) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured over temp range $296-473 \mathrm{~K}$ (flash photolysis-resonance fluorescence, Perry et al. 1977)
photooxidation $\mathrm{t}_{1 / 2}=8.021 \times 10^{3}-3.21 \times 10^{5} \mathrm{~h}$ in water, based on measured rate constant for reaction with OH radical in water (Güesten et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=1.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and residence time of 8.3 d , loss of $11.4 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=28 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Lyman et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=0.82 \times 10^{-9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=6.8 \mathrm{~d}$ in the atmosphere (Mill 1982)
$\mathrm{k}=(2.0 \pm 0.4) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water using $50-1000 \mathrm{mM} t-\mathrm{BuOH}$ as scavenger at pH 2.0 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{OH}}=(8.8 \pm 0.4) 1.45 \times 10^{-13} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 295 K (flash photolysis-resonance fluorescence, Wahner \& Zetzsch 1983)
$\mathrm{k}_{\mathrm{NO} 3}<2.3 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=1.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson et al. 1985)
$\mathrm{k}_{\mathrm{OH}} *=1.28 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=2.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.1.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=1.45 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K . (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=1.26 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $23.8^{\circ} \mathrm{C}$, with an atmospheric lifetime of 9.1 d (Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}} *=1.14 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured range $239-354 \mathrm{~K}$ (flash photolysis-resonance fluorescence, Witte et al. 1986)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=2.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.1.28 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(1.29 \pm 1.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K , measured range $234-438 \mathrm{~K}$ (flash photolysisresonance fluorescence, Wallington et al. 1987)
$\mathrm{k}_{\mathrm{O} 3}<0.01 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=1.28 \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}<3.2 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson \& Aschmann 1988)
$\mathrm{k}_{\mathrm{OH}} *=1.40 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=1.23 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=1.51 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).
Biodegradation:
$t_{1 / 2}=6 \mathrm{~d}$ in estuarine water (estimated, Lee \& Ryan 1976)
$\mathrm{t}_{1 / 2}$ (aq. aerobic) $=120-384 \mathrm{~h}$, based on seawater dieaway test data (Van der Linden 1978) and river dieaway data (Vaishnav \& Babeu, 1987; Howard et al. 1991)
$\mathrm{k}=4.58 \times 10^{-3} \mathrm{~h}^{-1}$ in water (Lee \& Ryan 1979; Mackay et al. 1985)
$\mathrm{k}=0.2 \mathrm{yr}^{-1}$ with $\mathrm{t}_{1 / 2}=110 \mathrm{~d}$ (Zoeteman et al 1981; Olsen \& Davis 1990)
$\mathrm{k}=0.5 \mathrm{~d}^{-1}$ significant degradation in favourable aerobic environment (Tabak et al. 1981; Mills et al. 1982)
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=2688-17280 \mathrm{~h}$, based on unacclimated aqueous anaerobic biodegradation screening test data (Horowitz et al. 1982; Howard et al. 1991)
$\mathrm{k}=0.12 \mathrm{~d}^{-1}$ in river water (estimated, Bartholomew \& Pfaender 1983; quoted, Battersby 1990)
$t_{1 / 2}=8.6 \mathrm{~d}$ in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991)
$\mathrm{k}=0.025 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=28 \mathrm{~d}$ in groundwater, $\mathrm{k}=0.044 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=16 \mathrm{~d}$ in Lester River with nutrient and microbial addition, and $\mathrm{k}=0.082 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=8 \mathrm{~d}$ in Superior harbor waters (Vaishnav \& Babeu 1987) $\mathrm{t}_{1 / 2}($ aerobic $)=5 \mathrm{~d}, \mathrm{t}_{1 / 2}($ anaerobic $)=110 \mathrm{~d}$ in natural waters (Capel \& Larson 1995)
$\mathrm{k}=0.58 \mathrm{~d}^{-1}$ associated with microbial population growth initially followed by a slower second phase with $\mathrm{k}=0.12 \mathrm{~d}^{-1}$ degradation by P. aeruginosa is a two-stage process (Kim et al. 2003).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Constants or Half-Lives:
$\mathrm{t}_{1 / 2}=0.5 \mathrm{~d}$ for elimination from eels, 0.5 d (Ogata \& Miyake 1978).
Half-Lives in the Environment:
Air: $t_{1 / 2} \geq 5.1 \mathrm{~h}$, based on a determined rate of disappearance in ambient LA basin air for reaction with OH radical at 300 K (Doyle et al. 1975);
$\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$, based on rate of disappearance for the reaction with OH radical (Darnall et al. 1976);
residence time of 8.3 d , loss of $11.4 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981);
$\mathrm{t}_{1 / 2}=50.1-501 \mathrm{~h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);
calculated lifetime of 9.1 d due to reaction with OH radical (Edney et al. 1986);
summer daylight lifetime of 115 h due to reaction with OH radical (Altshuller 1991);
calculated lifetimes of $9.4 \mathrm{~d},>4 \mathrm{yr}$ and $>4.5 \mathrm{yr}$ for reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$, respectively (Atkinson 2000).
Surface Water:
$\mathrm{t}_{1 / 2}=4.81 \mathrm{~h}$, based on evaporation loss at $25^{\circ} \mathrm{C}$ and 1 m depth of water (Mackay \& Leinonen 1975)
biodegradation $\mathrm{t}_{1 / 2} \sim 6 \mathrm{~d}$ in estuarine water (Lee \& Ryan 1976)
$\mathrm{t}_{1 / 2}=120-384 \mathrm{~h}$, based on unacclimated aerobic biodegradation half-life (Van der Linden 1978; Vaishnav \& Babeu 1987; Howard et al. 1991);
$t_{1 / 2}=23 \mathrm{~d}$ at $8-16^{\circ} \mathrm{C}$ in the spring, $\mathrm{t}_{1 / 2}=3.1 \mathrm{~d}$ at $20-22^{\circ} \mathrm{C}$ in the summer and $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ at $3-7^{\circ} \mathrm{C}$ in the winter, and $\mathrm{t}_{1 / 2}=6.9 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in September 9-15 from mesocosm experiments (Wakeham et al. 1983).
Ground water: $\mathrm{t}_{1 / 2} \sim 1$ yr from persistence observed in the groundwater of Netherlands (Zoeteman et al. 1981),
$\mathrm{t}_{1 / 2}=240-17280 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978;
Vaishnav \& Babeu 1987; Howard et al. 1991).
Soil: $\mathrm{t}_{1 / 2}=120-384 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978;
Vaishnav \& Babeu 1987; Howard et al. 1991);
$\mathrm{t}_{1 / 2}<10 \mathrm{~d}$ (Ryan et al. 1988);
$\mathrm{t}_{1 / 2}=365 \mathrm{~d}$, assumed first-order biological/chemical degradation in the soil (Jury et al. 1990);
disappearance $\mathrm{t}_{1 / 2}<2 \mathrm{~d}$ for test soils (Anderson et al. 1991).
Biota:

TABLE 3.1.1.1.1
Reported aqueous solubilities of benzene at various temperatures and reported temperature dependence equations

$$
\begin{aligned}
& \mathrm{R} \cdot \ln x=-\left[\Delta \mathrm{H}_{\mathrm{fus}} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{~T} / \mathrm{K}) \\
& \cdot \mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}_{1 / 2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d} \\
& \ln x=\mathrm{A}-\mathrm{B} / \mathrm{T}(\mathrm{~K}) \\
& \ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau, \text { where } \tau=\mathrm{T} / \mathrm{T}_{\mathrm{o}}, \mathrm{~T}_{\mathrm{o}}=298.15 \mathrm{~K}
\end{aligned}
$$

1. 

| Bohon \& Claussen 1951 |  | Arnold et al. 1958 |  | Alexander 1959 |  | Franks 1963 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-UV |  | shake flask-UV |  | shake flask-UV |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0.4 | 1741 | 4.5 | 1720 | 0.8 | 1840 | 17 | 1714 |
| 5.2 | 1810 | 4.9 | 1770 | 9.4 | 1790 | 22 | 1723 |
| 10 | 1800 | 5.0 | 1740 | 16.8 | 1770 | 25 | 1742 |
| 14.9 | 1770 | 6.7 | 1740 | 24 | 1800 | 29 | 1745 |
| 21 | 1790 | 9.0 | 1730 | 31 | 1830 | 32 | 1788 |
| 25.6 | 1790 | 12.5 | 1720 | 38 | 1920 | 35 | 1823 |
| 30.2 | 1843 | 15 | 1730 | 44.7 | 2030 | 40.5 | 1905 |
| 34.9 | 1877 | 20 | 1710 | 51.5 | 2140 | 42 | 1910 |
| 42.8 | 1998 | 20.6 | 1720 | 65.4 | 2340 | 44 | 1931 |
|  |  | 24.8 | 1710 |  |  | 46 | 1983 |
|  |  | 24.9 | 1740 |  |  | 51 | 2075 |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  | 27.3 | 1745 |  |  | 56 | 2183 |
| 25 | 2.42 | 30 | 1775 |  |  | 61 | 2305 |
| 12 | -2.30 | 30.9 | 1884 |  |  | 63 | 2352 |
| 17 | -0.25 | 45 | 1975 |  |  |  |  |
| 18 | 0 | 49.8 | 2044 |  |  |  |  |
| 22 | 1.34 | 54.5 | 2152 |  |  |  |  |
| 27 | 3.01 | 59.8 | 2265 |  |  |  |  |
| 32 | 4.435 | 64.8 | 2313 |  |  |  |  |
| 37 | 5.86 |  |  |  |  |  |  |

$$
\begin{gathered}
\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=2.27 \\
\text { at } 25^{\circ} \mathrm{C}
\end{gathered}
$$

2. 

| Leinonen 1972 |  | Udovenko \& Aleksandrova 1963 |  | Price 1973 |  | Bradley et al. 1973 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | polythermic method |  | shake flask-GC |  | shake flask-UV |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 4 | 1710 | 20 | 2100 | 25 | 1755 | 25 | 1830 |
| 5 | 1737 | 40 | 2270 | 55.3 | 3980 | 45 | 2160 |
| 5.4 | 1746 | 40.5 | 2480 | 84.7 | 6468 | 55 | 2380 |
| 6.1 | 1735 | 44.5 | 2590 |  |  |  |  |
| 7.0 | 1781 | 56.5 | 2880 |  |  |  |  |
| 10.3 | 1748 | 60 | 3000 |  |  |  |  |
| 13 | 1741 | 65 | 3190 |  |  |  |  |
| 16 | 1730 | 79.5 | 3730 |  |  |  |  |
| 19.1 | 1721 |  |  |  |  |  |  |
| 22.1 | 1739 |  |  |  |  |  |  |

TABLE 3.1.1.1.1 (Continued)
3.

| Brown \& Wasik 1974 |  | May et al. 1980, 1983 |  | Ben-Naim \& Wiff 1979 |  | Bittrich et al. 1979 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | generator column-HPLC/UV |  | shake flask-UV |  | shake flask-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 4,5 | 1840 | 0.2 | 1836 | 10 | 1625 | 20 | 1790 |
| 6.3 | 1850 | 6.2 | 1804 | 20 | 1734 | 40 | 2025 |
| 7.1 | 1810 | 11 | 1799 |  |  | 69 | 2442 |
| 9.0 | 1810 | 13 | 1770 |  |  |  |  |
| 11.8 | 1770 | 16.9 | 1762 |  |  |  |  |
| 12.1 | 1770 | 18.6 | 1767 |  |  |  |  |
| 15.1 | 1790 | 25.0 | 1790 |  |  |  |  |
| 17.9 | 1790 | 25.8 | 1819 |  |  |  |  |
| 20.1 | 1760 |  |  |  |  |  |  |

temp dependence eq. 2
given in May et al. 1978b and May 1980
S $\quad \mathrm{mg} / \mathrm{kg}$
a 0.0247
b $\quad-0.6838$
$\begin{array}{ll}\text { c } & 0.3166\end{array}$
d $\quad 1833$
4.

| Sanemasa et al. 1981 |  | Shaw 1989a (IUPAC) |  | Cooling et al. 1992 |  | Chen \& Wagner 1994a |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| vapor saturation-UV |  | recommended values |  | activity coefficient-GC |  | equilibrium flow cell-GC |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{2} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{s} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 15 | 1540 | 0 | 1690 | 20 | 1732 | 30 | 1840 |
| 25 | 1610 | 5 | 1800 | 30 | 1688 | 40 | 2014 |
| 35 | 1770 | 10 | 1780 | 40 | 1712 | 50 | 2213 |
| 45 | 1870 | 15 | 1760 | 50 | 1760 | 60 | 2452 |
|  |  | 20 | 1760 |  |  | 70 | 2713 |
|  |  | 25 | 1770 |  |  | 80 | 3033 |
|  |  | 30 | 1810 |  |  | 90 | 3472 |
|  |  | 35 | 1860 |  |  | 100 | 4123 |
| Sanemasa et al. 1982 |  | 40 | 1930 |  |  |  |  |
| vapor saturation-UV |  | 45 | 1990 |  |  | $\begin{gathered} \Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.69 \\ 25^{\circ} \mathrm{C} \end{gathered}$ |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | 50 | 2080 |  |  |  |  |
| 5 | 1620 | 55 | 2190 |  |  |  |  |
| 15 | 1580 | 60 | 2310 |  |  |  |  |
| 25 | 1620 | 65 | 2410 |  |  |  |  |
| 35 | 1710 | 70 | 2670 |  |  |  |  |
| 45 | 1800 |  |  |  |  |  |  |
|  |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=2.07$ |  |  |  |  |  |



FIGURE 3.1.1.1.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for benzene.

TABLE 3.1.1.1.2
Reported vapor pressures of benzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \cdot \mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}$
1.

| Stuckey \& Saylor 1940 |  | Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer |  | ebulliometry |  | summary of lit. data |  | ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 0 | 3509 | 14.548 | 7654 | -36.7 | 133.3* | 10.983 | 6397 |
| 12.5 | 6040 | 17.720 | 8962 | -19.6 | 266.6* | 14.575 | 7690 |
| 25 | 9960 | 20.504 | 10303 | -11.5 | 1333* | 17.697 | 8989 |
| 37.5 | 15800 | 23.270 | 11699 | -2.60 | 2666* | 20.028 | 11700 |
| 40 | 24240 | 26.886 | 13818 | 7.60 | 5333 | 23.271 | 11720 |
| 50 | 36050 | 31.004 | 16621 | 15.4 | 7999 | 26.908 | 13840 |
|  |  | 35.191 | 19922 | 26.1 | 13332 | 31.013 | 16631 |
| eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 30.078 | 23450 | 42.2 | 26664 | 35.207 | 19942 |
| A | 7.12491 | 44.284 | 28952 | 60.5 | 53323 | 39.095 | 23465 |
| B | 1323.06 | 49.066 | 34897 | 80.1 | 101325 | 44.294 | 28976 |
| C | 41.23 | 54.832 | 43320 |  |  | 49.084 | 34924 |
|  |  | 60.784 | 53652 |  | *solid | 54.852 | 43358 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 80.06 | 67.135 | 66753 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 5.5 | 60.803 | 53697 |
|  |  | 74.028 | 83717 |  |  | 67.148 | 66795 |
|  |  | 78.891 | 97601 |  |  | 74.035 | 83746 |
|  |  | 79.413 | 99197 |  |  | 78.903 | 97643 |
|  |  | 79.898 | 100689 |  |  | 79.424 | 99230 |

TABLE 3.1.1.1.2 (Continued)
1.

| Stuckey \& Saylor 1940 |  | Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer |  | ebulliometry |  | summary of lit. data |  | ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
|  |  | 80.442 | 102384 |  |  | 79.090 | 100722 |
|  |  | 80.922 | 106570 |  |  | 80.461 | 102460 |
|  |  |  |  |  |  | 80.948 | 104000 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |
|  |  | A | 6.89324 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | B | 1203.835 |  |  | A | 6.9210 |
|  |  | C | 219.924 |  |  | B | 1214.645 |
|  |  |  |  |  |  | B | 221.205 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 80.103 |  |  |  |  |
|  |  |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 80.099 |

2. 

| Bond \& Thodos 1960 |  | Ambrose et al. 1967 |  | Ambrose et al. 1970 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| compiled data |  | ebulliometry |  | compiled data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 7.565 | 5333 | 146.85 | 545800 | 46.85 | 32045 | -11.6 | 1333* |
| 39.093 | 23450 | 166.85 | 809200 | 66.85 | 66116 | -2.60 | 2666* |
| 67.15 | 66753 | 186.85 | 1156700 | 86.85 | 124180 | 3.0 | 4000* |
| 95.713 | 159987 | 206.85 | 1603700 | 106.85 | 215960 | 7.55 | 5333 |
| 110.015 | 231848 | 226.85 | 2166700 | 126.85 | 352460 | 11.80 | 6666 |
| 150.015 | 577419 | 246.85 | 2864400 | 146.85 | 545760 | 15.39 | 7999 |
| 180.015 | 1017250 | 266.85 | 3719300 | 166.85 | 809050 | 21.293 | 10666 |
| 240.015 | 2589787 | 286.85 | 4771700 | 186.85 | 1156600 | 26.075 | 13332 |
| 260.015 | 3376922 |  |  | 206.85 | 1603800 | 35.266 | 19998 |
|  |  | eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | 226.85 | 2166900 | 42.214 | 26664 |
| eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | A | 20.87440 | 246.85 | 2864000 | 47.868 | 33331 |
| A | 23.36128 | B | 2472.77 | 266.85 | 3718800 | 52.672 | 39997 |
| B | 2457.12 | C | 5.44671 | 286.85 | 4772600 | 60.611 | 53329 |
| C | 5.28840 | D | 1238 |  |  | 67.093 | 66661 |
| D | 1.56738 |  |  |  |  | 72.616 | 79993 |
|  |  |  |  |  |  | 77.454 | 93326 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 80.115 |  |  |  |  | 78.354 | 95991 |
|  |  |  |  |  |  | 79.236 | 98659 |
|  |  |  |  |  |  | 80.100 | 101325 |
|  |  |  |  |  |  | 25.0 | $12690$ |
|  |  |  |  |  |  |  | *solid |
|  |  |  |  |  |  | $\text { eq. } 2$ | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | $9.1064$ |
|  |  |  |  |  |  | B | $1885.9$ |
|  |  |  |  |  |  | C | $244.2$ |
|  |  |  |  |  |  |  | for liquid |
|  |  |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 6.90565 |
|  |  |  |  |  |  | B | 1211.033 |
|  |  |  |  |  |  | C | 220.790 |


4.

Ambrose 1981 (continued)

| ebulliometry |  | ebulliometry |  | gas saturation-GC |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| T/K | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  |  | t |  |  |
| 285.957 | 7014 | 297.769 | 12471 | -15.4 | 880 |
| 292.893 | 9903 | 302.633 | 15553 | -5.0 | 1750 |
| 298.684 | 13007 | 307.159 | 18957 | 10 | 6540 |
| 302.619 | 15545 | 308.384 | 19979 | 25 | 13100 |
| 304.302 | 16745 | 314.503 | 25716 | 40 | 26400 |
| 310.167 | 21539 | 319.907 | 31940 |  |  |
| 314.406 | 25665 | 324.512 | 38019 |  |  |
| 319.512 | 31444 | 329.473 | 45774 |  |  |

(Continued)

TABLE 3.1.1.1.2 (Continued)
4.

Ambrose 1981 (continued)
Liu \& Dickhut 1994

| ebulliometry |  | ebulliometry |  | gas saturation-GC |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| T/K | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 323.921 | 37264 | 333.842 | 53510 |  |  |
| 329.536 | 45876 | 338.144 | 62115 |  |  |
| 334.406 | 54580 | 342.687 | 77356 |  |  |
| 339.063 | 64081 | 347.828 | 85511 |  |  |
| 343.751 | 74940 | 352.112 | 97852 |  |  |
| 348.357 | 86959 | 352.617 | 99394 |  |  |
| 352.594 | 99320 | 352.955 | 100439 |  |  |
| 353.078 | 100816 | 358.109 | 117426 |  |  |
| 353.660 | 102633 | 362.258 | 132666 |  |  |
| 358.727 | 119597 | 367.239 | 152938 |  |  |
| 363.062 | 135783 | 372.175 | 175319 |  |  |
| 367.554 | 154281 | 377.584 | 202669 |  |  |
| 372.630 | 177510 |  |  |  |  |
| 377.875 | 204219 |  |  |  |  |
| 383.175 | 234260 |  |  |  |  |



FIGURE 3.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzene.

## TABLE 3.1.1.1.3

Reported Henry's law constants of benzene at various temperatures and reported temperature dependence equations

$$
\begin{align*}
& \ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1}\\
& \ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{2a}\\
& \ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{~m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{4a}\\
& \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{~T} / \mathrm{K})^{2}
\end{align*}
$$

$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
1.

| Brown \& Wasik 1974 |  | Green \& Frank 1979 |  | Leighton \& Calo 1981 |  | Sanemasa et al. 1981 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| headspace-GC |  | concentration ratio-UV |  | equilibrium cell-GC |  | vapor-liquid equilibrium |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{H / ( P a ~ m}{ }^{\mathbf{3} / \mathrm{mol})}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{\mathbf{3} / \mathrm{mol} \text { ) }}$ |
| 4.5 | 187.2 | 10 | 262 | 1.0 | 178 | 15 | 396 |
| 6.33 | 209.3 | 15 | 332 | 1.3 | 174 | 25 | 610 |
| 7.06 | 222.9 | 20 | 430 | 11 | 280 | 35 | 877 |
| 8.96 | 246.4 | 25 | 552 | 13 | 330 | 45 | 1267 |
| 11.75 | 289.9 | 30 | 688 | 21 | 470 |  |  |
| 12.1 | 295.3 |  |  | 33 | 482 |  |  |
| 15.1 | 346.8 | eq. 3 | $\mathrm{k}_{\mathrm{H}} / \mathrm{atm}$ | 27.2 | 597 | Sanemasa et al. 1982 |  |
| 17.93 | 391.6 | A | 8.58 | 25 | 554 | vapor liquid-equilibrium |  |
| 20.06 | 442.4 | B | 1852.308 |  |  | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
|  |  |  |  | eq. 3 | $\mathrm{k}_{\mathrm{H}} / \mathrm{atm}$ | 5 | 225 |
|  |  |  |  | A | 19.02 | 15 | 387 |
|  |  |  |  | B | 3964 | 25 | 608 |
|  |  |  |  |  |  | 35 | 905 |
|  |  |  |  |  |  | 45 | 1321 |

2. 

| Ashworth et al. 1988 |  | Robbins et al. 1993 |  | Perlinger et al. 1993 |  | Ettre et al. 1993 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EPICS-GC |  | static headspace-GC |  | headspace-GC |  | equil. headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) |
| 10 | 334 | 25 | 535 | 10 | 290 | 25 | 570 |
| 15 | 391 | 30 | 679 | 15 | 380 | 45 | 912 |
| 20 | 458 | 40 | 890 | 20 | 460 | 60 | 1220 |
| 25 | 535 | 45 | 1236 | 25 | 604 | 70 | 1668 |
| 30 | 730 | 50 | 1450 | 30 | 741 | 80 | 1767 |
| eq. 4 | $\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3}\right.$ |  |  |  |  | eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ |
| A | 5.534 |  |  |  |  | A | -2.1678537 |
| B | 3194 |  |  |  |  | B | 836.2228 |

3. 

| Dewulf et al. 1995 |  | Alaee et al. 1996 |  | Turner et al. 1996 |  | Peng \& Wan 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EPICS-GC |  | gas stripping-GC |  | vapor phase-equilibrium |  | headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 2.0 | 162 | 4 | 169 | 10 | 287 | 15 | 366 |
| 6.0 | 208 | 10 | 228 | 15 | 390 | 20 | 436 |
| 10 | 228 | 15 | 326 | 25 | 640 | 25 | 538 |

(Continued)

TABLE 3.1.1.1.3 (Continued)
3.

| Dewulf et al. 1995 |  | Alaee et al. 1996 |  | Turner et al. 1996 |  | Peng \& Wan 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EPICS-GC |  | gas stripping-GC |  | vapor phase-equilibrium |  | headspace-GC |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ | $t^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | $t /{ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 18.2 | 366 | 20.6 | 441 | 35 | 986 | 30 | 675 |
| 25 | 481 | 25.4 | 552 |  |  | 35 | 766 |
|  |  | 30.1 | 744 |  |  | 40 | 947 |
| eq. 1 | $\mathrm{K}_{\text {AW }}$ | 34.9 | 874 | eq. 5 | $\mathrm{K}_{\text {AW }}$ | 45 | 1053 |
| A | 10.577 |  |  | A | 0.0763 |  |  |
| B | 3640 |  |  | B | 0.00211 |  |  |
|  |  | enthalpy | volatilization: | C | 0.000162 | eq. 1 | $\mathrm{K}_{\text {AW }}$ |
|  |  | $\Delta \mathrm{H}_{\mathrm{vol}} /(\mathrm{kJ}$. | $\left.\mathrm{ol}^{-1}\right)=32.2$ |  |  | A | 7.15 |
|  |  |  | at $20^{\circ} \mathrm{C}$ |  |  | B | 1397 |
|  |  | eq. 1 | $\mathrm{K}_{\text {Aw }}$ |  |  |  |  |
|  |  | A | 11.5352 |  |  |  |  |
|  |  | B | 3873 |  |  |  |  |

4. 

| Bierwagen \& Keller 2001 |  | Görgényi et al. 2002 |  | Bakierowska \& T. 2003 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| SPME-GC |  | EPICS-SPME method |  | headspace-GC |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | $t /{ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | $t /{ }^{\circ} \mathrm{C}$ | H/(Pa m $\left.{ }^{3} / \mathrm{mol}\right)$ |
| 15 | 376 | 2 | 172.2 | 10 | 294 |
| 25 | 538 | 6 | 235.6 | 15 | 353.5 |
| 30 | 675 | 10 | 279.2 | 20 | 440 |
| 40 | 893 | 18 | 441.3 | 25 | 558 |
|  |  | 25 | 573.4 |  |  |
| eq. 1 | $\mathrm{K}_{\text {aw }}$ | 30 | 740.0 | Eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ |
| A | 8.1648 | 40 | 1033 | A | 11.663 |
| B | 2889.4 | 50 | 1429 | B | 3920 |
|  |  | 60 | 1844 |  |  |
|  |  | eq. 1 | $\mathrm{K}_{\text {AW }}$ |  |  |
|  |  | A | 10.01 |  |  |
|  |  | B | 3430.4 |  |  |



FIGURE 3.1.1.1.3 Logarithm of Henry's law constant versus reciprocal temperature for benzene.

TABLE 3.1.1.1.4
Reported octanol-water partition coefficients and octanolair partition coefficients of benzene at various temperatures

| $\log \mathrm{K}_{\text {Ow }}$ |  | $\boldsymbol{l o g} K_{\text {OA }}$ |  |
| :---: | :---: | :---: | :---: |
| Dewulf et al. 1999 |  | Gruber et al. 1997 |  |
| EPICS-GC, both phases |  | activity coefficient-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} \mathrm{K}_{\text {Ow }}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} \mathrm{K}_{\mathrm{OA}}$ |
| 2.2 | 1.973 | 20.29 | 2.9 |
| 6 | 1.961 | 30.3 | 2.71 |
| 10 | 2.053 | 40.4 | 2.56 |
| 14.1 | 2.01 | 50.28 | 2.42 |
| 18.7 | 2.04 |  |  |
| 24.8 | 1.974 |  |  |
| change in enthalpy: |  |  |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{OW}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=1.7 \\ & (-8.3 \text { to } 11.8) \end{aligned}$ |  |  |  |
| enthalpy of transfer |  |  |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{oc}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=8.1 \\ & (-1.9 \text { to } 18.2) \end{aligned}$ |  |  |  |



FIGURE 3.1.1.1.4 Logarithm of $K_{\text {Ow }}$ and $K_{O A}$ versus reciprocal temperature for benzene.

### 3.1.1.2 Toluene



Common Name: Toluene
Synonym: methyl benzene, phenylmethane, toluol, methylbenzol, methacide
Chemical Name: toluene
CAS Registry No: 108-88-3
Molecular Formula: $\mathrm{C}_{7} \mathrm{H}_{8}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}_{3}$
Molecular Weight: 92.139
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -94.95 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 110.63 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8669 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $106.3 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density) 118.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 37.99, $33.183 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
6.636 (Riddick et al. 1986) 6.62 (exptl., Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
37.15, 45.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or indicated. Additional data at other temperatures designated * are compiled at the end of this section):
$470 \quad\left(16^{\circ} \mathrm{C}\right.$, shake flask, Fühner, 1924)
$570 \quad\left(30^{\circ} \mathrm{C}\right.$, shake flask-interferometer, Gross \& Saylor 1931)
347 (residue-volume method, Booth \& Everson 1948)
530 (shake flask-UV, Andrews \& Keffer 1949)
500 (flask flask-UV, Klevens 1950)
627* (shake flask-UV, measured range $0.4-45.3^{\circ} \mathrm{C}$, Bohon \& Claussen 1951)
546 (shake flask-UV, Morrison \& Billett 1952)
550 (Dreisbach 1955)
595 (quoted, Deno \& Berkheimer 1960)
538 (shake flask-GC, McAuliffe 1963)
515 (shake flask-GC, McAuliffe 1966)
$479 \quad\left(21^{\circ} \mathrm{C}\right.$, shake flask-GC, Chey \& Calder 1972)
530* (shake flask-GC, measured range $5-45^{\circ} \mathrm{C}$, Pierotti \& Liabastre 1972)
547* (shake flask-UV, measured $25-55^{\circ} \mathrm{C}$, Bradley et al. 1973)
573* (shake flask-GC, Polak \& Lu 1973)
517 (shake flask-GC, Mackay \& Wolkoff 1973)
573* (headspace-GC, measured range $4.5-20.1^{\circ} \mathrm{C}$, Brown \& Wasik 1974)
627 (shake flask-UV, Vesala 1974)
520 (shake flask-GC, Mackay \& Shiu 1975)
534.8 (shake flask-GC, Sutton \& Calder 1975)

554 (shake flask-GC, Price 1976)
488; 563 (shake flask-titration, shake flask-cloud point, Sada et al. 1975)
$\begin{array}{ll}534 & \text { (shake flask-fluorescence, Schwarz 1977) } \\ 554 & \text { (shake flask-GC, Krzyzanowska \& Szeliga 1978) }\end{array}$
$\log x=626.526 /(\mathrm{T} / \mathrm{K})^{2}-4300.59 /(\mathrm{T} / \mathrm{K})+3.3585$, temp range $0-50^{\circ} \mathrm{C}$ (Ueda et al. 1978)
572, $587 \quad\left(10,20^{\circ} \mathrm{C}\right.$, shake flask-UV, Ben-Naim \& Wiff 1979)
660 (elution chromatography, Schwarz 1980)
732*, 739* ( $20^{\circ} \mathrm{C}$, exptl.-elution chromatography, shake flask-UV, Schwarz \& Miller 1980)
155 (shake flask-LSC, Banerjee et al. 1980)
507 (shake flask-GC, Rossi \& Thomas 1981)
557* (vapor saturation-UV spec., measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1981)
526* (vapor saturation-UV spec., measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
585 (generator column-HPLC/UV, Tewari et al. 1982b)
578 (generator column-HPLC/UV, Tewari et al. 1982c)
580 (generator column-HPLC/UV, Wasik et al. 1983)
524 (shake flask-HPLC/UV, Banerjee 1984)
521 (vapor saturation-UV spec., Sanemasa et al. 1984)
$\ln x=-185.1695+7348.55 /(\mathrm{T} / \mathrm{K})+26.34525 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $310-560 \mathrm{~K}$ (Heidman et al. 1985)
520 (shake flask-radiometry, Lo et al. 1986)
580 (shake flask-GC, Keeley et al. 1988)
538 (shake flask-GC, Coutant \& Keigley 1988)
530* (IUPAC recommended value, temp range $5-55^{\circ} \mathrm{C}$, Shaw 1989a)
599* $\quad\left(30^{\circ} \mathrm{C}\right.$, equilibrium flow cell-GC; measured range $30-100^{\circ} \mathrm{C}$ Chen \& Wagner 1994 b$)$
$\ln (1 / x)=-12.21+21.39 \cdot[(\mathrm{~T} / \mathrm{K}) / 591.8]^{-1}-3.572 \cdot[(\mathrm{~T} / \mathrm{K}) / 591.8]^{-2}$; temp range $303.15-373.15 \mathrm{~K}$ (equilibrium flow cell-GC, Chen \& Wagner 1994b)
$\ln x=12.21-21.39 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-1}+5.372 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-2}, \mathrm{~T}_{\mathrm{r}}=\mathrm{T}_{\mathrm{r}} \mathrm{T}_{\mathrm{c}}$, the reduced temp, system temp T divided by critical temp $\mathrm{T}_{\mathrm{c}}$ (Chen \& Wagner 1994c)
562.9 (shake flask-UV spectrophotometry, Poulson et al. 1999)
$\ln x=-46.05-7268.85 /(\mathrm{T} / \mathrm{K})-1.411 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
519* (shake flask-GC/FID, measured range $5-45^{\circ} \mathrm{C}$, Ma et al. 2001)
556* (vapor absorption technique-HPLC/UV, measured range $0.5-55^{\circ} \mathrm{C}$, Dohányosová et al. 2001)
558* (shake flask-UV, measured range $0-50^{\circ} \mathrm{C}$, Sawamura et al. 2001)
$\ln x=-221.739+9274.79 /(\mathrm{T} / \mathrm{K})+31.8721 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equation. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section):
$920^{*} \quad\left(0^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -9.70 to $0^{\circ} \mathrm{C}$, Linder 1931)
3786* ( Hg manometer measurements, Pitzer \& Scott 1943)
$\log (\mathrm{P} / \mathrm{mmHg})=-2866.53 /(\mathrm{T} / \mathrm{K})-6.7 \log (\mathrm{~T} / \mathrm{K})+27.6470$; temp range: $0-50^{\circ} \mathrm{C}$ (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer \& Scott 1943)
$6357^{*} \quad\left(35.366^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $35.366-111.509^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95337-1343.943 /\left(219.377+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35.4-111.5^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
$2666^{*} \quad\left(18.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -16.7 to $110.6^{\circ} \mathrm{C}$, Stull 1947)
$6386^{*} \quad\left(35.504^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $35.504-111.545^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95508-1345.087 /\left(219.516+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35.5-111.5^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
3792 (calculated from det. data, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95334-1343.943 /\left(219.377+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-200^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1333* $\left(6.375^{\circ} \mathrm{C}\right.$, compiled data, temp range $6.375-136.435^{\circ} \mathrm{C}$, Bond \& Thodos 1960$)$
$256200^{*} \quad\left(146.85^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $146.85-306.85^{\circ} \mathrm{C}$, Ambrose et al. 1967)
48898* ( $86.85^{\circ} \mathrm{C}$, compiled data, temp range $86.85-306.85^{\circ} \mathrm{C}$, Ambrose et al. 1970)
3792* (interpolated, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95464-1344.80 /\left(219.482+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range; $6.36-136.42^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9368.5 /(\mathrm{T} / \mathrm{K})]+8.3300$; temp range -92 to $-15^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8586.5 /(\mathrm{T} / \mathrm{K})]+8.719392$; temp range -26.7 to $319^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
2904* $\quad\left(19.99^{\circ} \mathrm{C}\right.$, differential capacitance gauge, measured range $0-49.26^{\circ} \mathrm{C}$, Munday et al. 1980)
$\log (\mathrm{P} / \mathrm{mmHg})=-5541.623 /(\mathrm{T} / \mathrm{K})+25.08047-0.01055321(\mathrm{~T} / \mathrm{K})$; temp range $0-49.26^{\circ} \mathrm{C}$ (differential capacitance gauge, Munday et al. 1980)
3560 (gas saturation-GC, Politzki et al. 1982)
$\log (\mathrm{P} / \mathrm{atm})=(1-383.737 / \mathrm{T}) \times 10^{\wedge}\left(0.837122-6.48791 \times 10^{4} \cdot \mathrm{~T}+5.91293 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 245.0-590.0 K (Cox vapor pressure eq., Chao et al. 1983)
$\log (\mathrm{P} / \mathrm{kPa})=6.08436-1347.62 /\left(219.787+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $35.37-111.5^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.37988-1575.007 /\left(249.372+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $86.85-306.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
3786 (Daubert \& Danner 1985)
3790 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95464-1344.80 /\left(219.48+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $6-137^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
3790 (headspace-GC, Hussam \& Carr 1985)
$\log (\mathrm{P} / \mathrm{kPa})=6.08540-1348.77 /\left(219.976+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
3800 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.08627-1349.122 /(-53.154+\mathrm{T} / \mathrm{K})$; temp range $308-386 \mathrm{~K}$ (liquid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1258-1376.61 /(-51.1+\mathrm{T} / \mathrm{K})$; temp range $210-219 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson $\&$ Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.12012-1374.901 /(-49.657+\mathrm{T} / \mathrm{K})$; temp range $383-445 \mathrm{~K}$ (liquid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.40815-1615.834 /(-15.897+\mathrm{T} / \mathrm{K})$; temp range $440-531 \mathrm{~K}$ (liquid, Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.65383-3153.235 /(188.566+\mathrm{T} / \mathrm{K})$; temp range $530-592 \mathrm{~K}$ (liquid, Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16273-1391.005 /(-48.974+\mathrm{T} / \mathrm{K})$; temp range $273-295 \mathrm{~K}$ (liquid, Antoine eq.-VI, Stephenson \& Malanowski 1987, selected, Shiu \& Ma 2000)
3090* $\quad\left(20.98^{\circ} \mathrm{C}\right.$, static method, measured range 199.22-402.21 K, Mokbel et al. 1998)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):

$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=-2.5323790+928.3536 /(\mathrm{T} / \mathrm{K})$; temp range $45-80^{\circ} \mathrm{C}$ (equilibrium headspace-GC measurements, Ettre et al. 1993)
631 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
660* (equilibrium headspace-GC, Perlinger et al. 1993)
652* (static headspace-GC, Robbins et al. 1993)
644 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
$676 \quad\left(23^{\circ} \mathrm{C}\right.$, gas stripping-IR, Nielsen et al. 1994)
555* (EPICS-GC/FID, Dewulf et al. 1995)
699 (EPICS-GC/FID, natural seawater with salinity of $35 \%$ Dewulf et al. 1995)
$\ln \mathrm{K}_{\mathrm{AW}}=-4064 /(\mathrm{T} / \mathrm{K})+0.00834 \cdot \mathrm{Z}+12.150$; with Z salinity $0-35.51$, temp range $2-35^{\circ} \mathrm{C}$, $(\mathrm{EPICS}-\mathrm{GC} / \mathrm{FID}$, Dewulf et al. 1995)
$541\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
684* (vapor-liquid equilibrium.-GC, Turner et al. 1996)
595 (gas stripping-GC, Altschuh et al. 1999)
605* (headspace equilibrium-GC, Peng \& Wan 1997)
$\ln \mathrm{K}_{\mathrm{AW}}=7.94-1621 /(\mathrm{T} / \mathrm{K})$; temp range $15-45^{\circ} \mathrm{C}$ ( headspace equilibrium-GC, Peng \& Wan 1997)
478 (headspace-GC, Peng \& Wan 1998)
$\ln \mathrm{K}_{\mathrm{AW}}=7.89-1565 /(\mathrm{T} / \mathrm{K})$; temp range $0-45^{\circ} \mathrm{C}$ (seawater with salinity of $36 \%$, headspace-GC, Peng \& Wan 1998)
637.2 (exponential saturator EXPSAT technique, Dohnal \& Hovorka 1999)
674.8 (modified EPICS method-GC, Ryu \& Park 1999)

652 (EPICS-GC, David et al. 2000)
644 (EPICS-static headspace method-GC/FID, Miller \& Stuart 2000)
959 (EPICS-GC, Ayuttaya et al. 2001)
$509 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=5.271-1745 /(\mathrm{T} / \mathrm{K})($ van $=\mathrm{t}$ Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
647.5* (EPICS-SPME, measured range $2-60^{\circ} \mathrm{C}$, Görgényi et al. 2002)
$\ln \mathrm{K}_{\mathrm{AW}}=11.25-3770.4 /(\mathrm{T} / \mathrm{K})$; temp range $2-60^{\circ} \mathrm{C}$ (EPICS-SPME method, Görgényi et al. 2002)
$556-574 \quad\left(27^{\circ} \mathrm{C}\right.$, solid-phase microextraction-GC, solute concn $0.47-19.21 \mathrm{mg} / \mathrm{L}$, measured range $15-40^{\circ} \mathrm{C}$, Cheng et al. 2003)
612* (headspace-GC, measured range $10-25^{\circ} \mathrm{C}$, Bakierowska \& Trzeszczyński 2003)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=11.926-3977 /(\mathrm{T} / \mathrm{K})$; temp range $10-25^{\circ} \mathrm{C}$, headspace-GC, Bakierowska \& Trzeszczyński 2003)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:
2.69 (shake flask-UV, Fujita et al. 1964; quoted, Hansch et al. 1968; Hansch et al. 1972)
2.11 (shake flask-UV, Rogers \& Cammarata 1969)
2.69, 2.73, 2.11, $2.80 \quad$ (Leo et al. 1971; Hansch \& Leo 1979)
2.21 (shake flask-LSC, Banerjee et al. 1980)
2.68 (shake flask-HPLC, Nahum \& Horvath 1980)
2.59 (HPLC-k' correlation, Hanai et al. 1981)
2.97 (HPLC-k' correlation, McDuffie 1981)
2.78 (HPLC-k' correlation, Hammers et al. 1982)
2.59 (HPLC-k' correlation, D'Amboise \& Hanai 1982)
2.65 (generator column-HPLC/UV, Tewari et al. 1982b,c)
2.62 (HPLC-k' correlation, Miyake \& Terada 1982)
2.65 (generator column-HPLC/UV, Wasik et al. 1983)
2.74 (HPLC- $\mathrm{k}^{\prime}$ correlation, Hafkanscheid \& Tomlinson 1983b)
2.11-2.80, 2.65 (range, mean; shake flask method, Eadsforth \& Moser 1983)
2.51-3.06, $2.88 \quad$ (range, mean; HPLC method, Eadsforth \& Moser 1983)
2.10 (shake flask, Platford 1979, 1983)
2.72 (HPLC-RV correlation, Garst \& Wilson 1984)
2.89 (HPLC-RT correlation, Rapaport \& Eisenreich 1984)
2.78 (HPLC/MS correlation, Burkhard et al. 1985)
3.00 (HPLC-k' correlation, De Kock \& Lord 1987)
2.65 (generator column-RP-LC, Schantz \& Martire 1987)
2.62 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
2.73 (recommended, Sangster 1989, 1993)
2.66, 2.69 (RP-HPLC capacity factor correlations, Sherblom \& Eganhouse 1988)
2.786 (shake flask/slow stirring-GC, De Brujin et al. 1989)
$2.63 \pm 0.05,2.786 \pm 0.005 \quad$ (shake flask/slow stirring, interlaboratory studies, Brooke et al. 1990)
2.76 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
2.73 (recommended, Hansch et al. 1995)
$2.77 \pm 0.02$ (HPLC-k' correlation, Poulson et al. 1997)
2.32* $\quad\left(24.8^{\circ} \mathrm{C}\right.$, EPICS-GC, measured range $2.2-24.8^{\circ} \mathrm{C}$, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:
$3.42^{*} \quad\left(20.29^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range 20.29-50.28 ${ }^{\circ} \mathrm{C}$, Gruber et al. 1997) 3.31 (head-space GC/FID both phases, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
1.12 (eels, Ogata \& Miyake 1978)
0.22 (Manila clam, Nunes \& Benville 1979)
0.62 (mussels, Geyer et al. 1982)
0.92 (goldfish, Ogata et al. 1984),
3.28, 2.58, $1.95 \quad$ (activated sludge, algae, fish, Freitag et al. 1985)
1.99 (S. capricornutum, Herman et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
2.39 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach \& Westall 1981)
2.27, 1.89 (ICN humic acid, ICN HA coated $\mathrm{Al}_{2} \mathrm{O}_{3}$, headspace equilibrium, Garbarnini \& Lion 1985)
2.28, 1.89 (Offutt AFB soil, Whitean AFB soil, headspace equilibrium, Garbarnini \& Lion 1985)
$1.91,1.13,1.19,2.18,2.09,-1.30,1.94 \quad$ (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, tannic acid, lignin, zein, cellulose, Aldrich humic acid, headspace equilibrium, Garbarnini \& Lion 1986)
2.18, 2.21, 2.43, 2.54 (Sapsucker Woods S.W. soil, S.W. ethyl ether extracted soil, humin, oxidized humin, headspace equilibrium, Garbarnini \& Lion 1986)
1.74. 2.13, $1.98 \quad$ (forest soil pH 5.6 , forest soil pH 4.2 , agricultural soil pH 7.4 , Seip et al. 1986)
2.0 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
1.70 (untreated Marlette soil A horizon, organic carbon OC $2.59 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.50, 2.39 (organic cations treated Marlette soil A horizon: HDTMA treated OC $6.48 \%$; DDTMA treated, OC $4.37 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.86, 2.86, 2.43 (organic cations treated Marlette soil $\mathrm{B}_{\mathrm{t}}$ horizon: HDTMA treated OC $3.72 \%$, DDTMA treated OC $1.98 \%$, NTMA treated, OC $1.18 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.59 (untreated St Clair soil $\mathrm{B}_{\mathrm{t}}$ horizon, OC $0.44 \%$, batch equilibrium, Lee et al. 1989)
3.03, 2.90 (organic cations HDTMA treated soils: St. Clair soil $B_{t}$ horizon OC $3.25 \%$; Oshtemo soil $B_{t}$ horizon OC $0.83 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.01 (aquifer material with $f_{\mathrm{OC}}=0.006$ and measured partition coeff. $\mathrm{K}_{\mathrm{P}}=0.61 \mathrm{~mL} / \mathrm{g}$., Abdul et al. 1990)
2.10, 2.26 (HPLC-k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
2.22, 2.16 (Captina silt loam, Mclaurin sandy loam, batch equilibrium, Walton et al. 1992)
2.10 (average of 5 soils, sorption isotherms by batch equilibrium method-GC, Xing et al. 1994)
2.21, 2.31, 2.21 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al. 1995)
2.17, 2.18 (RP-HPLC- $\mathrm{k}^{\prime}$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.12 (HPLC-screening method, Müller \& Kördel 1996)
2.23, 2.31, 2.33, 234, 2.40, 2.31, $2.34 \quad\left(2.3,3.8,6.2,8.0,13.5,18.6,25^{\circ} \mathrm{C}\right.$, natural sediment from River Leie, organic carbon $f_{\text {OC }}=4.12 \%$, EPICS-GC/FID, Dewulf et al. 1999)
$1.89,2.00,1.79$ (soils: organic carbon $\mathrm{OC} \geq 0.1 \%, \mathrm{OC} \geq 0.5 \%, 0.1 \leq \mathrm{OC}<0.5 \%$, average, Delle Site 2001)

Sorption Partition Coefficient, $\log \mathrm{K}_{\text {Ом }}$ :
1.39 (untreated Marlette soil A horizon, organic matter OM $5.18 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.30, 2.16 (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter $10.03 \%$; DDTMA treated, OM $5.18 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.74, 2.72, 2.28 (organic cations treated Marlette soil $\mathrm{B}_{\mathrm{t}}$ horizon: HDTMA treated OM $4.85 \%$, DDTMA treated OM $2.73 \%$, NTMA treated, OM $1.74 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.29 (untreated St Clair soil $B_{t}$ horizon, OM $0.88 \%$, batch equilibrium, Lee et al. 1989)
2.89; 2.74 (organic cations HDTMA treated soils: St. Clair soil $\mathrm{B}_{\mathrm{t}}$ horizon OM $4.38 \%$; Oshtemo soil $\mathrm{B}_{\mathrm{t}}$ horizon OM $1.12 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $\mathrm{t}_{1 / 2}=5.18 \mathrm{~h}$ from water depth of 1-m (Mackay \& Leinonen 1975; Haque et al. 1980);
$\mathrm{k}=0.043 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=16 \mathrm{~d}$ in spring at $8-16^{\circ} \mathrm{C}, \mathrm{k}=0.0463 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=1.5 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}$, $\mathrm{k}=0.053 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ for the periods when volatilization appears to dominate, and $\mathrm{k}=0.088 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=7.6 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$, in September 9-15, in marine mesocosm experiments (Wakeham et al. 1983);
evaporation $\mathrm{t}_{1 / 2} \sim 2.9 \mathrm{~d}$ from a river of $1-\mathrm{m}$ depth with wind speed of $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{s}$ at $20^{\circ} \mathrm{C}$ (Lyman et al. 1982);
estimated $\mathrm{t}_{1 / 2}=1$ and 4 d for evaporation from a river and lake, respectively (Howard 1990).
Photolysis: not environmentally significant or relevant (Mabey et al. 1982);
$\mathrm{k}=3.39 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with $\mathrm{HO} \cdot$ in the gas (Dilling et al. 1988); $t_{1 / 2}<0.25 \mathrm{~h}$ on silica gel under indoor artificial UV-light "continuous" condition (Söderström et al. 2004).
Oxidation: rate constant k ; for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:
$\mathrm{k}_{\mathrm{OH}}=(2.5 \pm 0.9) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=4.6 \mathrm{~h} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(0.450 \pm 0.045) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\left.\mathrm{O}{ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=5.78 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O} 3}=0.75 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=3.6 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$, with $\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ at room temp. (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}^{*}}=(6.40 \pm 0.64) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured over temp range 296-473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)
$\mathrm{k}_{\mathrm{OH}}=6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3} \leq 3 \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $300 \pm 1 \mathrm{~K}$ (Carter et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=6.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ and residence time of 1.9 d , loss of $40.9 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k} \ll 360 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=144 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for $\mathrm{RO}_{2}$ radical (Mabey et al. 1982)
$\mathrm{k}_{03}=160 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Lyman et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=3.5 \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1.6 \mathrm{~d}$ in the atmosphere (Mill 1982)
$\mathrm{k}=(14 \pm 3) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water at pH 1.7 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{O} 3}<1.0 \times 10^{-20} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ with a loss rate of $<0.0006 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=6.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.6 \mathrm{~d}^{-1}$ and $\mathrm{k}_{\mathrm{NO} 3}=3.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.0007 \mathrm{~d}^{-1}$ at room temp. (review, Atkinson \& Carter 1984)
$\mathrm{k}_{\mathrm{NO} 3}=1.8 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=6.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=5.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}\left(\mathrm{obs}\right.$.) $=5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=10-104 \mathrm{~h}$ (Atkinson 1985; Howard 1991)
$\mathrm{k}_{\mathrm{O} 3}<1.0 \times 10^{-20} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $<0.0006 \mathrm{~d}^{-1} ; \mathrm{k}_{\mathrm{OH}}=6.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.27 \mathrm{~d}^{-1}$ and $\mathrm{k}_{\mathrm{NO} 3}=3.6 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a loss rate of $0.0007 \mathrm{~d}^{-1}$ at room temp. (review, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=6.03 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=5.35 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $24.2^{\circ} \mathrm{C}$, with a calculated atmospheric lifetime $\tau=2.2 \mathrm{~d}$ (Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=5.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ obs. $)=6.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)
$\mathrm{k}_{\mathrm{NO} 3}=6.46 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=6.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{O} 3}<0.01 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=6.19 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=(7.8 \pm 1.5) \times 10^{-17}$ $\mathrm{cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate method, Atkinson \& Aschmann 1988)
$\mathrm{k}_{\mathrm{OH}} *=5.96 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
photooxidation $\mathrm{t}_{1 / 2}=10-104 \mathrm{~h}$, based on measured rate data for the vapor phase reaction with OH radicals in air; $\mathrm{t}_{1 / 2}(\mathrm{aq})=.321-1284 \mathrm{~h}$, based on measured rate data for hydroxyl radicals in aqueous solution (Howard et al. 1991)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=5.50 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992)
$\mathrm{k}_{\text {OH }}($ calc $)=4.79 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (based on molecular orbital calculations, Klamt 1993)
Hydrolysis: not aquatically significant (Callahan et al. 1979);
no hydrolyzable functional groups (Mabey et al. 1982).
Biodegradation:
$100 \%$ biodegraded after 192 h at $13^{\circ} \mathrm{C}$ with an initial concn of $2.22 \times 10^{-6} \mathrm{~L} / \mathrm{L}$ (Jamison et al. 1976)
$t_{1 / 2} \approx 90 \mathrm{~d}$ in uncontaminated estuarine water; and $\mathrm{t}_{1 / 2} \approx 30 \mathrm{~d}$ in oil polluted water (Lee 1977)
$\mathrm{k}=0.5 \mathrm{~d}^{-1}$, significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)
$\mathrm{k}=0.07 \mathrm{yr}^{-1}$ with $\mathrm{t}_{1 / 2}=39 \mathrm{~d}$ (Zoeteman et al. 1981; Olsen \& Davis 1990)
$\mathrm{t}_{1 / 2}($ aq. anaerobic $)=1344-5040 \mathrm{~h}$, based on anaerobic screening test data and anaerobic sediment grab sample data (Horowitz et al. 1982; Howard et al. 1991)
$\mathrm{t}_{1 / 2}=9.5 \mathrm{~d}$ in activated sludge (estimated, Freitag et al. 1985; quoted, Anderson et al. 1991)
$\mathrm{t}_{1 / 2}$ (aq. aerobic) $=: 96-528 \mathrm{~h}$, based on an acclimated seawater dieaway test (Howard et al. 1991)
$\mathrm{t}_{1 / 2}$ (aerobic) $=4 \mathrm{~d}, \mathrm{t}_{1 / 2}$ (anaerobic) $=56 \mathrm{~d}$ in natural waters (Capel \& Larson 1995)
$\mathrm{t}_{1 / 2}=31-220 \mathrm{~h}$ for toluene concn range from $0.5-200 \mu \mathrm{~g} / \mathrm{g}$ in sandy loam soil and degradation rate $\mathrm{k}=$ $1.76 \times 10^{-2}$ and $0.42 \mu \mathrm{~g} \mathrm{~g}^{-1} \mathrm{~h}^{-1}$ of soil for 0.5 and $5.0-\mathrm{g} / \mathrm{g}$, respectively; $\mathrm{t}_{1 / 2}=172$ and 165 h in sand and degradation rate $\mathrm{k}=1.05 \times 10^{-2}$ and $0.22 \mu \mathrm{~g} \mathrm{~g}^{-1} \mathrm{~h}^{-1}$ of soil for toluene concn 0.5 and $5 \mu \mathrm{~g} / \mathrm{g}$ respectively in sand (Davis \& Madsen 1996)
Biotransformation: $1.0 \times 10^{-7} \mathrm{~mL}^{\text {cell }}{ }^{-1} \mathrm{~h}^{-1}$ (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
$t_{1 / 2} \sim 1.4$ d elimination from eels in seawater (Ogata \& Miyake 1978).
Half-Lives in the Environment:
Air: $t_{1 / 2}=4.6 \mathrm{~h}$ in ambient air based on reaction with OH radical at $\sim 300 \mathrm{~K}$ (Doyle et al. 1975);
$\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ based on rate of disappearance for the reaction with hydroxyl radicals (Darnall et al. 1976)
photodecomposition $\mathrm{t}_{1 / 2}=6.8 \mathrm{~h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976)
residence time of 1.9 d , loss of $40.9 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
calculated lifetime $\tau=2.2 \mathrm{~d}$ due to reaction with OH radical (Edney et al. 1986)
summer daylight lifetime of 23 h due to reaction with OH radical (Altshuller 1991)
$\mathrm{t}_{1 / 2}=10-104 \mathrm{~h}$, based on photooxidation in air (Howard et al. 1991)
calculated lifetimes, $\tau=1.9 \mathrm{~d}, 1.9 \mathrm{yr}$ and $>4.5 \mathrm{yr}$ for reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$ respectively (Atkinson 2000).
Surface Water: $\mathrm{t}_{1 / 2}=5.55 \mathrm{~h}$, based on evaporative loss at $25^{\circ} \mathrm{C}$ and $1-\mathrm{m}$ depth of water (calculated, Mackay \& Leinonen 1975; Haque et al. 1980)
photooxidation $\mathrm{t}_{1 / 2}=321-1284 \mathrm{~h}$ in water, based on measured rate data for hydroxyl radical in aqueous solution (Dorfman \& Adams 1973; Howard et al. 1991)
$\mathrm{t}_{1 / 2}=16 \mathrm{~d}$ in spring at $6-16^{\circ} \mathrm{C}, \mathrm{t}_{1 / 2}=1.5 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}$, $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ when volatilization dominates and $\mathrm{t}_{1 / 2}=7.9 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in marine mesocosm experiments (Wakeham et al. 1983) $\mathrm{t}_{1 / 2}=96-528 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Ground water: $\mathrm{t}_{1 / 2} \approx 0.3 \mathrm{yr}$ from observed persistence in groundwater of Netherlands (Zoeteman et al. 1981); $\mathrm{t}_{1 / 2}=168-672 \mathrm{~h}$, based on unacclimated grab sample data of aerobic soil from groundwater aquifers (Wilson et al. 1983; Swindoll et al. 1987; Howard et al. 1991).
Soil: $\mathrm{t}_{1 / 2}<10 \mathrm{~d}$ (Ryan et al. 1988)
$\mathrm{t}_{1 / 2}=5 \mathrm{~d}$ assumed first-order biological/chemical degradation in soil (Jury et al. 1990);
reported lit. $t_{1 / 2}=0.1-1.7 \mathrm{~d}$ and 7 d in soil, measured disappearance $\mathrm{t}_{1 / 2}<2.0 \mathrm{~d}$ from test soils (Anderson et al. 1991)
$\mathrm{t}_{1 / 2}=96-528 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
$\mathrm{t}_{1 / 2}=31,57,96$ and 220 h with toluene concn range from $0.5,5,50$ and $200 \mu \mathrm{~g} / \mathrm{g}$ in sandy loam soil, $\mathrm{t}_{1 / 2}=$ 172 and 165 h with toluene concn 0.5 and $5 \mu \mathrm{~g} / \mathrm{g}$, respectively, in sand (Davis \& Madsen 1996).
Biota: $t_{1 / 2}=10 \mathrm{~h}$ clearance from fish (Neely 1980).

TABLE 3.1.1.2.1
Reported aqueous solubilities of toluene at various temperatures and reported enthalpy of solution 1.

| Bohon \& Claussen 1951 |  | Pierotti \& Liabastre 1972 |  | Bradley et al. 1973 |  | Brown \& Wasik 1974 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-GC |  | shake flask-UV |  | headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathbf{m}^{-3}$ |
| 0.4 | 658 | 5 | 634 | 25 | 547 | 25 | 573 |
| 3.6 | 646 | 10 | 632 | 45 | 722 | 4.5 | 612 |
| 10 | 628 | 20 | 661 | 55 | 860 | 6.3 | 601 |
| 11.2 | 624 | 25 | 630 |  |  | 7.1 | 586 |
| 14.9 | 623 | 35 | 672 |  |  | 9 | 587 |
| 15.9 | 621 | 45 | 672 |  | 1973 | 11.8 | 573 |
| 25 | 627 |  |  |  | k-GC | 12.1 | 575 |
| 25.6 | 625 | $\Delta_{\text {sol }} \mathrm{H} /(\mathrm{l}$ | $\left.{ }^{-1}\right)=1.50$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | 15.1 | 569 |
| 30 | 640 |  |  |  |  | 17.9 | 577 |
| 30.2 | 642 |  |  | 0 | 724 | 20.1 | 566 |
| 35.2 | 657 |  |  | 25 | 573 |  |  |
| 42.8 | 701 |  |  |  |  | $\Delta_{\text {sol }} \mathrm{H} /$ | $\left.{ }^{-1}\right)=4.70$ |
| 45.3 | 717 |  |  |  |  |  |  |
| $\Delta_{\text {sol }} \mathrm{H} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |  |  |  |  |  |  |  |
| $25^{\circ} \mathrm{C}$ | 2.3 |  |  |  |  |  |  |
| $2^{\circ} \mathrm{C}$ | -3.93 |  |  |  |  |  |  |
| $7^{\circ} \mathrm{C}$ | -3.01 |  |  |  |  |  |  |
| $12^{\circ} \mathrm{C}$ | -1.38 |  |  |  |  |  |  |
| $17^{\circ} \mathrm{C}$ | 0 |  |  |  |  |  |  |
| $22^{\circ} \mathrm{C}$ | 0.962 |  |  |  |  |  |  |
| $27^{\circ} \mathrm{C}$ | 3.22 |  |  |  |  |  |  |
| $32^{\circ} \mathrm{C}$ | 4.435 |  |  |  |  |  |  |
| $37^{\circ} \mathrm{C}$ | 5.73 |  |  |  |  |  |  |
| $42^{\circ} \mathrm{C}$ | 7.15 |  |  |  |  |  |  |

2. 

| Ben-Naim \& Wiff 1979 |  | Schwarz \& Miller 1980 |  | Sanemasa et al. 1981 |  | Shaw 1989a (IUPAC) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-UV |  | vapor saturation-UV |  | recommended values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 10 | 572 | 10 | 777 | 15 | 533 | 0 | 690 |
| 20 | 587 | 20 | 739 | 25 | 557 | 5 | 630 |
|  |  | 30 | 754 | 35 | 587 | 10 | 590 |
|  |  |  |  | 45 | 635 | 20 | 570 |
|  |  |  |  |  |  | 25 | 530 |
|  |  | Elution | matography |  | $\left.\mathrm{mol}^{-1}\right)=3.70$ | 30 | 590 |
|  |  | t/ $/{ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |  |  | 40 | 640 |
|  |  | 10 | 758 |  |  | 45 | 660 |


3.

| Chen \& Wagner 1994b |  | Ma et al. 2001 |  | Dohányosová et al. 2001 |  | Sawamura et al. 2001 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| equilibrium flow cell-GC |  | shake flask-GC/FID |  | vapor absorption-HPLC/UV |  | shake flask-UV |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{s} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{s} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 30 | 599 | 5 | 540 | 0.5 | 563 | 0 | 583.5 |
| 40 | 609 | 15 | 516 | 5 | 552 | 5 | 670 |
| 50 | 650 | 25 | 519 | 15 | 542 | 10 | 558 |
| 60 | 737 | 35 | 555 | 25 | 556 | 15 | 553 |
| 70 | 875 | 45 | 632 | 35 | 590 | 20 | 553 |
| 80 | 1013 |  |  | 45 | 632 | 25 | 558 |
| 90 | 1187 |  |  | 55 | 704 | 30 | 573.8 |
| 100 | 1371 |  |  | $\begin{aligned} & \Delta \mathrm{H}_{\text {sol }}\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.0 \\ & \text { at } 25^{\circ} \mathrm{C} \end{aligned}$ |  | 35 | 589.1 |
| $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=0.37 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  |  |  |  |  | 40 | 614.7 |
|  |  |  |  |  |  | 45 | 640.3 |
|  |  |  |  |  |  | 50 | 676.6 |



FIGURE 3.1.1.2.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for toluene.

TABLE 3.1.1.2.2
Reported vapor pressures of toluene at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{align*}
& \log P=A-B /(T / K)  \tag{1}\\
& \log P=A-B /\left(C+t /{ }^{\circ} C\right)  \tag{2a}\\
& \log P=A-B /(C+T / K) \\
& \log P=A-B /(T / K)-C \cdot \log (T / K)  \tag{4}\\
& \log P=A-B /(T / K)-C \cdot \log (T / K)+D \cdot P /(T / K)^{2}  \tag{5}\\
& \log P=A-B /(T / K)-C \cdot(T / K)+D \cdot(T / K)^{2} \tag{6}
\end{align*}
$$

$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
(3)
1.

| Pitzer \& Scott 1943 | Stull 1947 |  | Willingham et al. 1945 |  | Forziati et al. 1949 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer | summary of literature data |  | ebulliometry |  | ebulliometry |  |
| $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | $\mathbf{t}^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
| 0900 | -16.7 | 133.3 | 35.366 | 6357 | 35.504 | 6386 |
| 12.51920 | -4.40 | 666.6 | 39.343 | 7654 | 39.437 | 7690 |
| $25 \quad 3786$ | 6.40 | 1333 | 42.810 | 8962 | 45.997 | 10328 |
| $37.5 \quad 7026$ | 18.4 | 2666 | 45.948 | 10303 | 48.894 | 11719 |
| $50 \quad 12266$ | 31.8 | 5333 | 48.867 | 11700 | 52.848 | 13840 |
|  | 40.3 | 7999 | 52.802 | 13818 | 57.315 | 16632 |
| eq. $4 \quad \mathrm{P} / \mathrm{mmHg}$ | 51.9 | 13332 | 57.293 | 16621 | 61.869 | 19942 |
| A 27.6470 | 69.5 | 26664 | 61.851 | 19929 | 66.107 | 23473 |
| B 2866.53 | 89.5 | 53329 | 66.079 | 23450 | 71.758 | 28976 |
| $\begin{array}{ll}\text { C } & 6.70\end{array}$ | 110.6 | 101325 | 71.738 | 28952 | 76.965 | 34924 |
|  |  |  | 76.942 | 34897 | 83.230 | 43359 |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=38.137 \\ & \text { at } 298 \mathrm{~K} \end{aligned}$ | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -95 | 83.202 | 43320 | 89.659 | 53697 |
|  |  |  | 89.667 | 53600 | 96.580 | 66795 |
|  |  |  | 96.559 | 66672 | 104.052 | 83748 |
|  |  |  | 104.037 | 83717 | 109.328 | 97644 |
| Linder 1931 |  |  | 109.312 | 97603 | 109.894 | 99232 |
| mercury manometer |  |  | 109.879 | 99200 | 110.420 | 100724 |
| $\mathbf{t}^{\circ} / \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ |  |  | 110.403 | 100690 | 111.018 | 102460 |
| -9.70 470.6 |  |  | 110.991 | 102385 | 111.545 | 104000 |
| -8.70 502.6 |  |  | 111.509 | 103930 |  |  |


| -7.20 | 556 |  |  |  |  |
| :--- | :--- | :---: | :---: | :---: | :---: |
| -4.40 | 664 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| -4.35 | 666.6 | A | 6.95337 | A | 6.95508 |
| -3.70 | 706.6 | B | 1343.943 | B | 1345.087 |
| -3.50 | 714.6 | C | 219.377 | C | 219.516 |
| -2.75 | 742.6 |  |  |  |  |
| 0 | 920 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 110.623 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 110.626 |

2. 

| Bond \& Thodos 1960 |  | Ambrose et al. 1970 |  | Zwolinski \& Wilhoit 1971 |  | Munday et al. 1980 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| compiled data |  | compiled data |  | selected values |  | differential capacitance gauge |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 6.375 | 1333 | 86.85 | 48898 | 6.36 | 1333 | 0.0 | 901.3 |
| 46.748 | 10666 | 106.85 | 90907 | 18.38 | 2666 | 6.06 | 1309 |
| 90.682 | 53643 | 126.85 | 157180 | 26.03 | 4000 | 10.2 | 1763 |
| 120.585 | 133322 | 146.85 | 255940 | 31.76 | 5333 | 19.99 | 3706 |
| 136.435 | 199984 | 166.85 | 396580 | 36.394 | 6666 | 29.89 | 4864 |
|  |  | 186.85 | 589400 | 40.308 | 7999 | 39.60 | 7743 |


| TABLE 3.1.1.2.2 (Continued) |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Bond \& Thodos 1960 |  | Ambrose et al. 1970 |  | Zwolinski \& Wilhoit 1971 |  | Munday et al. 1980 |  |
| compiled data |  | compiled data |  | selected values |  | differential capacitance gauge |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathbf{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | $t /{ }^{\circ} \mathrm{C}$ | P/Pa |
| eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | 206.85 | 845520 | 46.733 | 10666 | 49.26 | 11870 |
| A | 24.27652 | 226.85 | 1176900 | 51.940 | 13332 |  |  |
| B | 2690.80 | 246.85 | 1597500 | 61.942 | 19998 | eq. 6 | $\mathrm{P} / \mathrm{mmHg}$ |
| C | 5.45371 | 266.85 | 2122500 | 69.498 | 26664 | A | 25.08047 |
| D | 2.04294 | 286.85 | 2768000 | 75.644 | 33331 | B | 5541.623 |
|  |  | 306.85 | 3556300 | 80.863 | 39997 | C | 0.01055321 |
| bp/ ${ }^{\circ} \mathrm{C}$ | 110.64 |  |  | 89.484 | 53329 | D | 0 |
|  |  |  |  | 96.512 | 66661 |  |  |
|  |  |  |  | 102.511 | 79993 | Mokbel et al. 1998 |  |
| Ambrose et al. 1967 |  |  |  | 107.575 | 93326 | static method* |  |
| ebulliometry |  |  |  | 108.733 | 95992 | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |  |  | 109.689 | 98659 | 199.22 | $1.051 \times 10^{-3}$ |
| 146.85 | 256200 |  |  | 110.625 | 101325 | 215.91 | $7.660 \times 10^{-3}$ |
| 166.85 | 396600 |  |  | 25.0 | 3792 | 234.88 | $5.001 \times 10^{-2}$ |
| 186.85 | 589400 |  |  |  |  | 254.64 | 0.252 |
| 206.85 | 845400 |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 110.625 | 274.01 | 0.956 |
| 226.85 | 1177100 |  |  |  |  | 278.99 | 1.305 |
| 246.85 | 1597700 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 284.17 | 1.764 |
| 266.85 | 2122200 |  |  | A | 6.95464 | 294.13 | 3.090 |
| 286.85 | 2767600 |  |  | B | 1344.80 | 304.06 | 5.145 |
| 306.85 | 3556800 |  |  | C | 219.482 | 314.03 | 8.257 |
|  |  |  |  |  |  | 324.06 | 12.836 |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  | 334.04 | 19.275 |
| eq. 5 | P/bar |  |  | at $25^{\circ} \mathrm{C}$ | 37.99 | 344.02 | 28.185 |
| A | 20.17980 |  |  | at bp | 33.18 | 353.98 | 40.016 |
| B | 2640.04 |  |  |  |  | 363.95 | 55.744 |
| C | 5.14885 |  |  |  |  | 372.03 | 71.857 |
| D | 1434 |  |  |  |  | 382.08 | 96.602 |
| $1 \mathrm{bar}=1 \times 10^{5} \mathrm{~Pa}$ |  |  |  |  |  | 392.10 | 127.860 |
|  |  |  |  |  |  | 402.21 | 166.405 |
|  |  |  |  |  |  | *complete list see ref. |  |



FIGURE 3.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for toluene.

TABLE 3.1.1.2.3
Reported Henry's law constants of toluene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
1.

| Brown \& Wasik 1974 |  | Leighton \& Calo 1981 |  | Sanemasa et al. 1981 |  | Schoene \& S. 1985 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| head space-GC |  | equilibrium cell-GC |  | vapor liquid-equilibrium |  | headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m³/mol) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m³/mol) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m $\left.{ }^{3} / \mathrm{mol}\right)$ |
| 4.5 | 179 | 1.0 | 222 | 15 | 382 | 20 | 634 |
| 6.33 | 204 | 1.3 | 236 | 25 | 628 | 36.9 | 670 |
| 7.06 | 218 | 12.4 | 373 | 35 | 979 | 41.5 | 680 |
| 8.96 | 244 | 12.5 | 361 | 45 | 1404 | 46 | 690 |
| 11.75 | 294 | 17.9 | 459 |  |  |  |  |
| 12.1 | 299 | 19.1 | 525 |  |  | eq. 1 | $\mathrm{K}_{\text {AW }}$ |
| 15.1 | 259 | 22.7 | 565 | Sanem | a et al. 1982 | A | 6.90 |
| 17.93 | 414 | 23 | 625 | vapor-li | id equilibrium | B | 2194 |
| 20.06 | 474 |  |  | t/ ${ }^{\circ} \mathrm{C}$ | H/Pa m ${ }^{3} / \mathrm{mol}$ |  |  |
|  |  | eq. 3 | $\mathrm{k}_{\mathrm{H}} / \mathrm{atm}$ |  |  |  |  |
|  |  | A | 18.46 | 15 | 396 |  |  |
|  |  | B | 3751 | 25 | 664 |  |  |
|  |  |  |  | 35 | 1060 |  |  |
|  |  |  |  | 45 | 1571 |  |  |

2. 

| Ashworth et al. 1988 |  | Kolb et al. 1992 |  | Ettre et al. 1993 |  | Perlinger et al. 1993 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EPICS-GC |  | static headspace-GC |  | headspace-GC |  | equil. headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 10 | 386 | 40 | 933 | 45 | 1116 | 10 | 293 |
| 15 | 499 | 60 | 1565 | 60 | 1489 | 15 | 390 |
| 20 | 562 | 70 | 1915 | 70 | 1877 | 20 | 499 |
| 25 | 651 | 80 | 2312 | 80 | 2427 | 25 | 660 |
| 30 | 819 |  |  |  |  | 30 | 838 |
|  |  | eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ | eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ |  |  |
| eq 4 a | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ | A | 7.61 | A | -2.532379 |  |  |
| A | 5.133 | B | 2647 | B | 928.3536 |  |  |
| B | 3024 |  |  |  |  |  |  |

3. 

| Robbins et al. 1993 |  | Dewulf et al. 1995 |  | Turner et al. 1996 |  | Peng \& Wan 1997 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static headspace-GC |  | EPICS-GC |  | vapor phase-equilibrium |  | headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 25 | 652 | 2.0 | 175 | 11 | 376 | 15 | 391 |
| 30 | 835 | 6.0 | 203 | 15 | 460 | 20 | 475 |
| 40 | 1086 | 10 | 250 | 25 | 684 | 25 | 605 |


| TABLE 3.1.1.2.3 (Continued) |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Robbins et al. 1993 |  | Dewulf et al. 1995 |  | Turner et al. 1996 |  | Peng \& Wan 1997 |  |
| static headspace-GC |  | EPICS-GC |  | vapor phase-equilibrium |  | headspace-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ |
| 45 | 1351 | 18.2 | 424 | 35 | 1202 | 30 | 774 |
| 50 | 1450 | 25 | 555 |  |  | 35 | 984 |
|  |  |  |  | eq. 5 | $\mathrm{K}_{\text {AW }}$ | 40 | 1104 |
| eq. 4 a | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ | eq 1 | $\mathrm{K}_{\text {AW }}$ | A | 0.115 | 45 | 1309 |
| A | 7.14 | A | 12.40 | B | 0.00474 |  |  |
| B | 3689 | B | 4064 | C | 0.000466 | eq. 1 | $\mathrm{K}_{\text {AW }}$ |
|  |  |  |  |  |  | A | 7.94 |
|  |  |  |  |  |  | B | 1621 |
| 4. |  |  |  |  |  |  |  |
| Görgényi et al. 2002 |  | Bakierowska \& T. 2003 |  |  |  |  |  |
| EPICS-SPME method |  | headspace-GC |  |  |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |  |  |  |  |
| 2.0 | 169.3 | 10 | 288 |  |  |  |  |
| 6.0 | 238.2 | 15 | 358 |  |  |  |  |
| 10 | 304.9 | 20 | 467 |  |  |  |  |
| 18 | 476.9 | 25 | 612 |  |  |  |  |
| 25 | 647.5 |  |  |  |  |  |  |
| 30 | 822.4 | eq. 2 | $1 / \mathrm{K}_{\text {AW }}$ |  |  |  |  |
| 40 | 1214 | A | 11.926 |  |  |  |  |
| 50 | 1758 | B | 3977 |  |  |  |  |
| 60 | 2286 |  |  |  |  |  |  |
| eq. 1 | $\mathrm{K}_{\text {AW }}$ |  |  |  |  |  |  |
| A | 11.25 |  |  |  |  |  |  |
| B | 3770.4 |  |  |  |  |  |  |



FIGURE 3.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for toluene.

TABLE 3.1.1.2.4
Reported octanol/water partition coefficients and octanol-air partition coefficients of toluene at various temperatures

| $\log K_{\text {ow }}$ |  | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\mathrm{OA}}$ |  |
| :---: | :---: | :---: | :---: |
| Dewulf et al. 1999 |  | Gruber et al. 1997 |  |
| EPICS-GC, both phases |  | GC det'd activity coeff. |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} K_{\text {ow }}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\log \mathrm{K}_{\text {OA }}$ |
| 2.2 | 2.316 | 20.29 | 3.42 |
| 6 | 2.405 | 30.3 | 3.2 |
| 10 | 2.464 | 40.4 | 3.03 |
| 14.1 | 2.38 | 50.28 | 2.86 |
| 18.7 | 2.41 |  |  |
| 24.8 | 2.32 |  |  |
|  | change |  |  |
|  | -1) $=-1.0$ |  |  |
|  | to 13.9) |  |  |




FIGURE 3.1.1.2.4 Logarithm of $K_{O W}$ and $K_{O A}$ versus reciprocal temperature for toluene.

### 3.1.1.3 Ethylbenzene



Common Name: Ethylbenzene
Synonym: phenylethane, ethylbenzol
Chemical Name: ethylbenzene
CAS Registry No: 100-41-4
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{10}, \mathrm{C}_{2} \mathrm{H}_{5} \mathrm{C}_{6} \mathrm{H}_{5}$
Molecular Weight: 106.165
Melting Point $\left({ }^{\circ} \mathrm{C}\right)$ : -94.96 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
136.2 (Weast 1982-83; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.867 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$122.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density, McAuliffe 1966; Stephenson \& Malanowski 1987)
140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 42.25, $35.2\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.184 (Riddick et al. 1986)
9.16 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
51.43, 52.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$140 \quad\left(15^{\circ} \mathrm{C}\right.$, shake flask, Fühner 1924)
168 (shake flask-UV, Andrews \& Keefer 1950)
175 (shake flask-UV, Klevens 1950)
208* (shake flask-UV, measured range $0.4-42.8^{\circ} \mathrm{C}$, Bohon \& Claussen 1951)
165 (shake flask-UV, Morrison \& Billett 1952)
159 (shake flask-GC, McAuliffe 1963)
152 (shake flask-GC, McAuliffe 1966)
177* (shake flask-GC, Polak \& Lu 1973)
180* (shake flask-GC, measured range $4.5-20.1^{\circ} \mathrm{C}$, Brown \& Wasik 1974)
203 (shake flask-UV, Vesala 1974)
161 (shake flask-GC, Sutton \& Calder 1975)
131 (shake flask-GC, Price 1976)
131 (shake flask-GC, Krzyzanowska \& Szeliga 1978)
203, $212\left(10,20^{\circ} \mathrm{C}\right.$, shake flask-UV, Ben-Naim \& Wiff 1979)
$208^{*}, 184^{*}\left(20^{\circ} \mathrm{C}\right.$, elution chromatography, shake flask-UV, measured range $10-30^{\circ} \mathrm{C}$, Schwarz \& Miller 1980)
181* (vapor saturation-UV, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1981)
169* (vapor saturation-UV, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
172 (generator column-HPLC/UV, Tewari et al. 1982a)
187 (generator column-HPLC/UV, Tewari et al. 1982c)
166 (HPLC-k' correlation, converted from $\gamma_{\mathrm{w}}$, Hafkenscheid \& Tomlinson 1983a)
187 (generator column-HPLC/UV, Wasik et al. 1983)
172 (vapor saturation-UV, Sanemasa et al. 1984)

192* (generator column-HPLC/UV, measured range $10-45^{\circ} \mathrm{C}$, Owens et al. 1986)
172 (shake flask-purge and trap-GC, Coutant \& Keigley 1988)
169* (IUPAC recommended value, temp range $0-100^{\circ} \mathrm{C}$, Shaw1989b)
$170^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, equilibrium flow cell-GC, measured range $30-100^{\circ} \mathrm{C}$, Chen \& Wagner 1994c)
$\ln x=11.59-20.52 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-1}+4.750 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-2} ; \mathrm{T}_{\mathrm{r}}=\mathrm{T}^{2} \mathrm{~T}_{\mathrm{c}}$, the reduced temp, system temp T divided by critical temp $\mathrm{T}_{\mathrm{c}}$, temp range $303.15-373.15 \mathrm{~K}$ (equilibrium flow cell-GC, Chen \& Wagner 1994c)
$\ln x=-30.799+3986.26 /(\mathrm{T} / \mathrm{K})+7.9095 \times 10^{-5} \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
170* (vapor absorption technique-HPLC/UV, measured range $0.5-55^{\circ} \mathrm{C}$, Dohányosová et al. 2001)
170* (shake flask-UV, measured range $0-50^{\circ} \mathrm{C}$, Sawamura et al. 2001)
$\ln x=-263.220+11024.75 /(\mathrm{T} / \mathrm{K})+37.8858 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
209.3* $\quad\left(0^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -11.6 to $0^{\circ} \mathrm{C}$, Linder 1931)

1546* $\quad\left(30^{\circ} \mathrm{C}, \mathrm{Hg}\right.$ manometer, measured range $10-50^{\circ} \mathrm{C}$, Rintelen 1937)
$\log (\mathrm{P} / \mathrm{mmHg})=22.90283-2847.75 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})$; temp range $4-75^{\circ} \mathrm{C}$ (vapor pressure eq. from manometer measurements, Stuckey \& Saylor 1940)
$6277^{*} \quad\left(56.589^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $56.589-137.124^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.94998-1419.315 /\left(212.611+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $56.6-137.1^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
1333* $\quad\left(25.9^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
8399* $\quad\left(63.3^{\circ} \mathrm{C}\right.$, static- Hg manometer, measured range $63.3-135.9^{\circ} \mathrm{C}$, Buck et al. 1949)
$6398^{*} \quad\left(56.689^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $56.689-137.16^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95904-1425.464 /\left(213.345+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $56.7-137.2^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=-3225 /(\mathrm{T} / \mathrm{K})-7.553 \cdot \log (\mathrm{~T} / \mathrm{K})+30.49$; temp range $80-120^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
1276(extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95719-1424.255 /\left(213.206+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range: $45-190^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
133800* $\quad\left(146.85^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $146.85-326.85^{\circ} \mathrm{C}$, Ambrose et al. 1967)
1270* (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95719-1424.255 /\left(213.206+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $25.88-163.47^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9303.3 /(\mathrm{T} / \mathrm{K})]+7.809470$; temp range -9.8 to $326.5^{\circ} \mathrm{C}$, (Antoine eq., Weast 1972-73)
$9585^{*} \quad\left(66.031^{\circ} \mathrm{C}\right.$, comparative ebulliometry, measured range $66.031-176.953^{\circ} \mathrm{C}$, Osborn \& Scott 1980)
$\log (\mathrm{P} / \mathrm{atm})=(1-409.229 / \mathrm{T}) \times 10^{\wedge}\left(0.859833-6.85948 \times 10^{4} \cdot \mathrm{~T}+5.94439 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 243.2-615.0 K (Cox vapor pressure eq., Chao et al. 1983)

1270, 1265 (extrapolated-Antoine eq., Boublik et al. 1984; quoted, Howard 1989)
$\log (\mathrm{P} / \mathrm{kPa})=6.08206-1425.305 /\left(213.415+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range: $25.88-92.7^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.0785-1421.653 /\left(212.816+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $56.6-137.12^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
1268 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95719-1424.255 /\left(213.21+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $26-164^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
1300 (selected value., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.09280-1431.71 /\left(214.099+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
1266 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.06991-1416.922 /(-69.716+\mathrm{T} / \mathrm{K})$; temp range $298-420 \mathrm{~K}$ (liquid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.10898-1445.262 /(-57.128+\mathrm{T} / \mathrm{K})$; temp range $409-459 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.36656-1665.991 /(-26.716+\mathrm{T} / \mathrm{K})$; temp range $457-554 \mathrm{~K}$ (liquid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.49119-3056.747 /(159.496+\mathrm{T} / \mathrm{K})$; temp range $549-617 \mathrm{~K}$ (liquid, Antoine eq.-IV, Stephenson \& Malanowski 1987)
1280, 283 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=36.1998-3.3402 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.7970 \cdot \log (\mathrm{~T} / \mathrm{K})-1.1467 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+2.5758 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $178-617 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
559.1* $\quad\left(20.06^{\circ} \mathrm{C}\right.$, headspace-GC, Brown \& Wasik 1974)

757 (calculated-bond contribution, Hine \& Mookerjee 1975)
879 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}, \mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, reported as exptl., Hine \& Mookerjee 1975)
854 (batch stripping-GC, Mackay et al. 1979; quoted, Howard 1989)
734* (vapor-liquid equilibrium-GC, Sanemasa et al. 1981)
797* (vapor-liquid equilibrium.-GC, Sanemasa et al. 1982)
653 (gas stripping-GC, Warner et al. 1987)
798* (EPICS-GC/FID, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=11.92-4994 /(\mathrm{T} / \mathrm{K})$, temp range $10-30^{\circ} \mathrm{C}$, EPICS measurements, Ashworth et al. 1988)
815 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
756 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
660* (equilibrium headspace-GC, Perlinger et al. 1993)
788* (static headspace-GC, Robbins et al. 1993)
397 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
669* (EPICS-GC/FID, measured range $2-25^{\circ} \mathrm{C}$, Dewulf et al. 1995)
302, $838\left(6.0,25^{\circ} \mathrm{C}\right.$, EPICS-GC/FID, natural seawater with salinity of $35 \%$, Dewulf et al. 1995)
$\ln \mathrm{K}_{\mathrm{AW}}=-4567 /(\mathrm{T} / \mathrm{K})+0.01047 \cdot \mathrm{Z}+14.001$; with Z salinity $0-35.5 \%$, temp range: $2-35^{\circ} \mathrm{C}$ (EPICS-GC/FID, Dewulf et al. 1995)
$602\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
895 (vapor-liquid equilibrium.-GC, Turner et al. 1996)
629 (EPICS-static headspace method-GC/FID, Miller \& Stuart 2000)
943.2 (modified EPICS method-GC, Ryu \& Park 1999)
$583 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=6.541-2100 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
$1173-1273\left(27^{\circ} \mathrm{C}\right.$, equilibrium headspace-GC, solute concn $0.43-18.66 \mathrm{mg} / \mathrm{L}$, measured range $300-315 \mathrm{~K}$, Cheng et al. 2003)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ at $25^{\circ} \mathrm{C}$ :

| 3.15 | (shake flask-UV, Hansch et al. 1968; Hansch \& Leo 1979; Hansch \& Leo 1985) |
| :--- | :--- |
| 3.13 | (calculated-fragment const., Rekker 1977) |
| 3.12 | (HPLC-k' correlation, Hanai et al. 1981) |
| 3.12 | (HPLC-k' correlation, D'Amboise \& Hanai 1982) |
| 3.26 | (HPLC-k' correlation, Hammers et al. 1982) |
| 3.15 | (generator column-HPLC/UV, Tewari et al. 1982a) |
| 3.13 | (generator column-HPLC/UV, Tewari et al. 1982c) |
| 3.16 | (HPLC-k' correlation, Miyake \& Terada 1982) |
| 3.24 | (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983b) |
| 3.13 | (generator column-HPLC/UV, Wasik et al. 1983) |
| 3.13 | (generator column-RP-LC, Schantz \& Martire 1987) |
| $3.13,3.21$ | (RP-HPLC capacity factor correlations, Sherblom \& Eganhouse 1988) |
| 3.15 | (recommended, Sangster 1989, 1993) |
| 3.15 | (recommended, Hansch et al. 1995) |
| $3.32,3.32, ~ 3.53,3.51$ |  |
| under isocratic conditions, Makovsakya et al. 1995) |  |

3.05 (RP-HPLC-RT correlation, short ODP column, Donovan \& Pescatore 2002)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated
$3.85,3.62,3.41,3.24 \quad\left(20.29,30.3,40.4,50.28^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\circ}$ in octanol, Gruber et al. 1997)
3.72, 3.698 (interpolated value from exptl value of Gruber et al. 1997, calculated using measured $\gamma^{\infty}$ in pure octanol by Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
0.67 (clams, exposed to water-soluble fraction of crude oil, Nunes \& Benville 1979; selected, Howard 1989)
2.16 (fish, calculated, Lyman et al. 1982; quoted, Howard 1989)
2.67 (microorganisms-water, calculated-K ${ }_{\text {Ow }}$, Mabey et al., 1982)
1.19 (goldfish, Ogata et al. 1984)
1.20, 1.19 (fish: calculated, correlated, Sabljic 1987b)
2.31 (S. capricornutum, Herman et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
1.98 (soil, sorption isotherm, Chiou et al. 1983)
2.41 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
2.30 (RP-HPLC-k' correlation, cyanopropyl column, Hodson \& Williams 1988)
2.03 (untreated Marlette soil A horizon, organic carbon OC $2.59 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.83, 2.61 (organic cations treated Marlette soil A horizon: HDTMA treated OC 10.03\%; DDTMA treated, OC $4.37 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.13 (untreated Marlette soil $\mathrm{B}_{\mathrm{t}}$ horizon, organic carbon OC $0.30 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.23, 3.12, 2.58 (organic cations treated Marlette soil $\mathrm{B}_{\mathrm{t}}$ horizon: HDTMA treated OC 3.72\%, DDTMA treated OC $1.98 \%$, NTMA treated, OC $1.18 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.26, 2.38 (untreated soils: St. Clair soil $B_{t}$ horizon OC $0.44 \%$; Oshtemo soil $B_{t}$ horizon OC $0.11 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
3.37, 3.19 (organic cations HDTMA treated soils: St. Clair soil $B_{t}$ horizon OC $3.25 \%$; Oshtemo soil $B_{t}$ horizon OC $0.83 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.27, 2.05 (Riddles soil: top layer pH 5.0 , below top layer pH 5.3 , batch equilibrium, Boyd et al. 1990)
2.52, 2.47 (RP-HPLC-k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
2.35, 2.40, 2.42 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al.1995)
2.51, 2.51 (RP-HPLC- $\mathrm{k}^{\prime}$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.32 (HPLC-screening method, Müller \& Kördel 1996)
$2.49,2.73,2.65,2.73,2.77,2.732 .74 \quad\left(2.3,3.8,6.2,8.0,13.5,18.6,25^{\circ} \mathrm{C}\right.$, natural sediment from River Leie, organic carbon $f_{\mathrm{OC}}=4.12 \%$, EPICS-GC/FID, Dewulf et al. 1999)
2.04, 2.18, 1.90 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%$, $\mathrm{OC} \geq 0.5 \%, 0.1 \leq \mathrm{OC}<0.5 \%$, average, Delle Site 2001)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OM}}$ :
1.98 (Woodburn silt loam soil, $1.9 \%$ organic matter, equilibrium isotherm-GC, Chiou et al. 1983)
1.04 (untreated Marlette soil A horizon, organic matter OM 5.18\%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
$1.89,1.81$ (organic cations treated Marlette soil A horizon: HDTMA treated, organic matter 10.03\%; DDTMA treated, OM 5.18\%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.53, 2.46, 2.08 (organic cations treated Marlette soil $\mathrm{B}_{\mathrm{t}}$ horizon: HDTMA treated OM 4.85\%, DDTMA treated OM $2.73 \%$, NTMA treated, OM $1.74 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.56, 2.53 (organic cations HDTMA treated soils: St. Clair soil $B_{t}$ horizon OM 4.38\%; Oshtemo soil $B_{t}$ horizon OM $1.12 \%$, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, k, or Half-lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: rate constants: $\mathrm{k}=0.035 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=20 \mathrm{~d}$ in spring at $8-16^{\circ} \mathrm{C}, \mathrm{k}=0.331 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.1 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{k}=0.054 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ for the periods when volatilization
appears to dominate, and $\mathrm{k}=0.097 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=7.1 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in September 9-15, in marine mesocosm experiments (Wakeham et al. 1983);
$\mathrm{t}_{1 / 2} \sim 3.1 \mathrm{~h}$ of evaporation from a river of 1 m depth with wind speed $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{s}$ at $20^{\circ} \mathrm{C}$ (Lyman et al. 1982; quoted, Howard 1989).
Photolysis: not environmentally significant or relevant (Mabey et al. 1982).
Oxidation: rate constant k ; for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated ${ }^{*}$, see reference:
$\mathrm{k}_{\text {OH }}=(4.8 \pm 1.0) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=4.8 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-24 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{t}_{1 / 2} \approx 15 \mathrm{~h}$ in water, probably not important as aquatic fate (Callahan et al. 1979)
$\mathrm{k}_{\text {OH }}=8.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and residence time of 1.4 d , loss of $51 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k} \ll 360 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $720 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for $\mathrm{RO}_{2}$ radical (Mabey et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=4.4 \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1.3 \mathrm{~d}$ in the atmosphere (Mill 1982)
$\mathrm{k}_{\mathrm{o} 3}=340 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Lyman et al. 1982)
$\mathrm{k}=(14 \pm 4) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water using $100 \mathrm{mM} t$-BuOH as scavenger at pH 2.0 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{OH}}=7.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=8.56-85.6 \mathrm{~h}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=6.47 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}\left(\mathrm{obs}\right.$.) $=7.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\text {OH }}=7.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $\sim 298 \mathrm{~K}$ (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.06 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ ( molecular orbital calculations, Klamt 1993)
Hydrolysis: not aquatically significant (Callahan et al. 1979);
no hydrolyzable functional groups (Mabey et al. 1982)
Biodegradation:
$100 \%$ biodegraded after 192 h at $13^{\circ} \mathrm{C}$ with an initial concn of $1.36 \times 10^{-6} \mathrm{~L} / \mathrm{L}$ (Jamison et al. 1976)
$\mathrm{t}_{1 / 2}($ aq. aerobic $)=72-240 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991);
$\mathrm{t}_{1 / 2}($ aq. anaerobic $)=4224-5472 \mathrm{~h}$, based on anaerobic groundwater die-away test data (Wilson et al. 1986; Howard et al. 1991)
$\mathrm{k}=0.5 \mathrm{~d}^{-1}$, significant degradation under favourable conditions in an aerobic environment (Tabak et al. 1981; Mills et al. 1982)
$t_{1 / 2} \sim 2 \mathrm{~d}$ degradation by established microorganisms depending on body of water and its temperature (Howard 1989)
$\mathrm{k}=0.07 \mathrm{yr}^{-1}$ with $\mathrm{t}_{1 / 2}=37 \mathrm{~d}$ (Olsen \& Davis 1990).
Biotransformation: $3 \times 10^{-9} \mathrm{~mL}^{2}$ cell-1 $\mathrm{h}^{-1}$ (Mabey et al. 1982).
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.24-24 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976);
photodecomposition $\mathrm{t}_{1 / 2}=5.0 \mathrm{~h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976);
residence time of 1.4 d , loss of $51 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
summer daylight lifetime $\tau=20 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991);
$\mathrm{t}_{1 / 2}=8.56-85.6 \mathrm{~h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991).
Surface Water: $\mathrm{t}_{1 / 2}=5-6 \mathrm{~h}$ (Callahan et al. 1979), based on the estimated evaporative loss of toluene at $25^{\circ} \mathrm{C}$ and 1 m depth of water (Mackay \& Leinonen 1975);
$t_{1 / 2}=20 \mathrm{~d}$ in spring at $6-16^{\circ} \mathrm{C}, \mathrm{t}_{1 / 2}=2.1 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ and $\mathrm{t}_{1 / 2}=7.1 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in marine mesocosm experiments (Wakeham et al. 1983);
$\mathrm{t}_{1 / 2}=72-240 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991).
Ground water: $\mathrm{t}_{1 / 2}=144-5472 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991);
$\mathrm{t}_{1 / 2} \sim 0.3 \mathrm{yr}$ from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).

Soil: $t_{1 / 2}=72-240 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991); $\mathrm{t}_{1 / 2}<10 \mathrm{~d}$ (Ryan et al. 1988).

Biota:

TABLE 3.1.1.3.1
Reported aqueous solubilities of ethylbenzene at various temperatures
1.

| Bohon \& Claussen 1951 |  | Polak \& Lu 1973 |  | Brown \& Wasik 1974 |  | Ben-Naim \& Wiffb 1979 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-GC |  | headspace-GC |  | shake flask-UV |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0.4 | 219 | 0 | 197 | 4.5 | 196 | 10 | 203 |
| 5.2 | 213 | 25 | 177 | 6.3 | 192 | 20 | 212 |
| 20.7 | 207 |  |  | 7.1 | 186 |  |  |
| 21.2 | 207 |  |  | 9 | 187 |  |  |
| 25 | 208 |  |  | 11.8 | 181 |  |  |
| 25.6 | 209 |  |  | 12.1 | 183 |  |  |
| 30.2 | 211 |  |  | 15.1 | 180 |  |  |
| 34.9 | 221 |  |  | 17.9 | 184 |  |  |
| 42.8 | 231 |  |  | 20.1 | 180 |  |  |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  | $\Delta \mathrm{H}_{\text {sol }}$ | $\left.\mathrm{l}^{-1}\right)=11.9$ |  |  |
| $25^{\circ} \mathrm{C}$ | 1.6 |  |  |  |  |  |  |
| $2^{\circ} \mathrm{C}$ | -3.98 |  |  |  |  |  |  |
| $7{ }^{\circ} \mathrm{C}$ | -2.74 |  |  |  |  |  |  |
| $12^{\circ} \mathrm{C}$ | -1.63 |  |  |  |  |  |  |
| $17^{\circ} \mathrm{C}$ | -0.343 |  |  |  |  |  |  |
| $22^{\circ} \mathrm{C}$ | -0.167 |  |  |  |  |  |  |
| $27^{\circ} \mathrm{C}$ | 1.97 |  |  |  |  |  |  |
| $32^{\circ} \mathrm{C}$ | 3.615 |  |  |  |  |  |  |
| $37^{\circ} \mathrm{C}$ | 7.36 |  |  |  |  |  |  |

2. 

| Schwarz \& Miller 1980 | Sanemasa et al. 1981 | Owens et al. 1986 |  | Shaw 1989b (IUPAC) |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV | vapor saturation-UV | generator column-HPLC/UV |  | recommended values |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| $10 \quad 180$ | 15176 | 10 | 197 | 0 | 200 |
| 20184 | $25 \quad 181$ | 14 | 192 | 10 | 180 |
|  | $35 \quad 194$ | 17 | 189 | 20 | 181 |
| elution chromatography | $45 \quad 215$ | 18 | 183 | 25 | 169 |
| 10211 |  | 19 | 178 | 30 | 190 |
| 20208 | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=3.60$ | 20 | 188 | 40 | 200 |
|  | at $25^{\circ} \mathrm{C}$ | 21 | 183 | 50 | 220 |
|  |  | 22 | 182 | 60 | 250 |
|  | Sanemasa et al. 1982 | 23.5 | 186 | 70 | 280 |
|  | vapor saturation-UV | 25 | 192 | 80 | 330 |
|  | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | 25.8 | 186 | 90 | 390 |
|  |  | 28 | 185.5 | 100 | 460 |
|  | $15 \quad 160$ | 30 | 188.7 |  |  |
|  | $25 \quad 169$ | 35 | 193 |  | $\left.\mathrm{l}^{-1}\right)=2.1$ |

TABLE 3.1.1.3.1 (Continued)

| Schwarz \& Miller 1980 |  | Sanemasa et al. 1981 |  | Owens et al. 1986 |  | Shaw 1989b (IUPAC) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | vapor saturation-UV |  | $\underline{\text { generator column-HPLC/UV }}$ |  | recommended values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathrm{m}^{-3}$ |
|  |  | 35 | 176 | 40 | 205 | at $25^{\circ} \mathrm{C}$ |  |
|  |  | 45 | 196 | 45 | 211.4 |  |  |
|  |  | $\begin{gathered} \Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.90 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  | $\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=1.30$ |  |  |  |
|  |  |  |  |  |  |  |  |

3. 

| Chen \& Wagner 1994c |  | Dohányosová et al. 2001 |  | Sawamura et al. 2001 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| equil. flow cell-GC |  | vapor abs-HPLC/UV |  | shake flask-UV |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{\mathbf{- 3}}$ |
| 30 | 170 | 0.5 | 169 | 0 | 190.8 |
| 40 | 172 | 5 | 167 | 5 | 182 |
| 50 | 198 | 15 | 167 | 10 | 175 |
| 60 | 240 | 25 | 170 | 15 | 170 |
| 70 | 291 | 35 | 177 | 20 | 169 |
| 80 | 353 | 45 | 188 | 25 | 170 |
| 90 | 410 | 55 | 213.5 | 30 | 173.8 |
| 100 | 504 | $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.0 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  | 35 | 179.8 |
| $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=1.30 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  |  |  | 40 | 188.1 |
|  |  | 45 | 196.9 |
|  |  | 50 | 208 |



FIGURE 3.1.1.3.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for ethylbenzene.

TABLE 3.1.1.3.2
Reported vapor pressures of ethylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
1.

| Linder 1931 | Willingham et al. 1945 |  | Stull 1947 |  | Buck et al. 1949 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer | ebulliometry |  | summary of literature data |  | static-Hg manometer |  |
| $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -11.6 74.7 | 56.589 | 6277 | -9.8 | 133.3 | 63.3 | 8399 |
| -1.20 184 | 60.796 | 7654 | 13.9 | 266.6 | 67.7 | 10133 |
| 0209.3 | 64.463 | 8962 | 25.9 | 1333 | 75.2 | 13999 |
|  | 67.775 | 10303 | 38.6 | 2666 | 82.6 | 18665 |
|  | 70.862 | 11699 | 52.8 | 5333 | 91.6 | 25998 |
|  | 75.027 | 13919 | 61.8 | 7999 | 99 | 33864 |
|  | 79.777 | 16608 | 74.1 | 13332 | 108.1 | 45596 |
| Rintelin et al. 1937 | 84.599 | 19924 | 92.7 | 26664 | 112.7 | 52662 |
| mercury manometer | 89.071 | 23450 | 113.8 | 53323 | 117.6 | 60928 |
| t/ ${ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ | 95.056 | 28954 | 136.2 | 101325 | 120.5 | 66128 |
| 10387 | 100.561 | 34897 |  |  | 125.6 | 75460 |
| $30 \quad 1546$ | 107.183 | 43320 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -94.9 | 129.3 | 85060 |
| $50 \quad 4613$ | 114.02 | 53654 |  |  | 135.9 | 100792 |
|  | 121.312 | 66755 |  |  |  |  |
|  | 129.221 | 83717 |  |  | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |
|  | 134.8 | 97603 |  |  | A | 3225 |
|  | 135.399 | 99199 |  |  | B | 7.553 |
| Stuckey \& Saylor 1940 | 135.954 | 100690 |  |  | C | 30.49 |
| static-Hg manometer | 136.574 | 102385 |  |  | temp range: |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | 137.124 | 103903 |  |  | $80-120^{\circ} \mathrm{C}$ |  |
| measured $4-75^{\circ} \mathrm{C}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |
| eq. $4 \quad \mathrm{P} / \mathrm{mmHg}$ | A | 6.94998 |  |  |  |  |
| A 22.9028 | B | 1419.315 |  |  |  |  |
| B 2857.75 | C | 212.611 |  |  |  |  |
| C 5 | bp/ ${ }^{\circ} \mathrm{C}$ |  |  |  |  |  |
|  |  | 136.187 |  |  |  |  |
| bp/ ${ }^{\circ} \mathrm{C} \quad 136.32$ |  |  |  |  |  |  |

2. 

| Forziati et al. 1949 |  | Ambrose et al. 1967 |  | Zwolinski \& Wilhoit 1971 |  | Osborn \& Scott 1980 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | ebulliometry |  | selected values |  | comparative ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 56.689 | 6398 | 146.85 | 133800 | 25.88 | 1333 | 66.031 | 9585 |
| 60.887 | 7690 | 166.85 | 216100 | 38.6 | 2666 | 69.091 | 10887 |
| 64.51 | 8990 | 186.85 | 332500 | 46.69 | 4000 | 72.167 | 12339 |
| 67.827 | 10330 | 206.85 | 492000 | 52.75 | 5333 | 75.258 | 13956 |
| 70.891 | 11720 | 226.85 | 703300 | 57.657 | 6666 | 78.254 | 15748 |
| 75.054 | 13840 | 246.85 | 976500 | 61.789 | 7999 | 81.465 | 17734 |

TABLE 3.1.1.3.2 (Continued)

| Forziati et al. 1949 |  | Ambrose et al. 1967 |  | Zwolinski \& Wilhoit 1971 |  | Osborn \& Scott 1980 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | ebulliometry |  | selected values |  | comparative ebulliometry |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa |
| 79.791 | 16633 | 266.85 | 1321500 | 68.596 | 10666 | 84.587 | 19933 |
| 83.619 | 19944 | 286.85 | 1751100 | 74.105 | 13332 | 90.869 | 25023 |
| 89.09 | 23474 | 306.85 | 2279100 | 84.687 | 19998 | 97.199 | 31177 |
| 95.074 | 28978 | 326.85 | 2924900 | 92.68 | 26664 | 103.575 | 38565 |
| 100.675 | 34925 |  |  | 99.182 | 33331 | 110.001 | 47375 |
| 107.21 | 43360 | eq. 5 | P/bar | 104.703 | 39997 | 116.474 | 57817 |
| 114.046 | 53698 | A | 21.956 | 113.823 | 53329 | 122.998 | 70120 |
| 121.331 | 66796 | B | 2923.84 | 121.266 | 66661 | 129.571 | 84532 |
| 129.234 | 83749 | C | 5.67301 | 127.603 | 79993 | 136.193 | 101325 |
| 134.815 | 97645 | D | 1772 | 133.152 | 93326 | 142.863 | 120790 |
| 135.413 | 99235 |  |  | 134.185 | 95991 | 149.587 | 143240 |
| 135.969 | 100725 |  |  | 135.196 | 98659 | 156.356 | 169020 |
| 136.602 | 102462 |  |  | 135.164 | 101325 | 163.174 | 198490 |
| 137.16 | 103999 |  |  | 25 | 1266.6 | 170.038 | 232020 |
|  |  |  |  |  |  | 176.953 | 270030 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
| A | 6.959 |  |  | A | 6.95719 | data fitted to | constant |
| B | 1425.46 |  |  | B | 1424.255 | vapor pressu |  |
| C | 213.345 |  |  | C | 213.206 |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 136.186 |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 136.186 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |  |  |  |
|  |  |  |  | at $25^{\circ} \mathrm{C}$ | 42.25 |  |  |
|  |  |  |  | at bp | 35.56 |  |  |



FIGURE 3.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for ethylbenzene.

## TABLE 3.1.1.3.3

Reported Henry's law constants of ethylbenzene at various temperatures and temperature dependence equations

| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (1) | $\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (2) | $\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| $\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (4) | $\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| $\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$ | (5) |  |

1. 

| Brown \& Wasik 1974 |  | Sanemasa et al. 1981 vapor-liquid equilibrium |  | Sanemasa et al. 1982 vapor-liquid equilibrium |  | Ashworth et al. 1988 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| head space-GC |  |  |  |  | PICS-GC |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |  |  | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 4.5 | 187.5 | 15 | 459 | 15 | 418 | 10 | 330 |
| 6.33 | 217.2 | 25 | 797 | 25 | 734 | 15 | 457 |
| 7.06 | 235.1 | 35 | 1339 | 35 | 1211 | 20 | 609 |
| 8.96 | 265 | 45 | 1436 | 45 | 1436 | 25 | 798 |
| 11.75 | 329 |  |  |  |  | 30 | 1064 |
| 12.1 | 333.6 |  |  |  |  |  |  |
| 15.1 | 409.7 |  |  |  |  | eq. 4 a | $\mathrm{H} /(\mathrm{atm} \mathrm{m} 3 / \mathrm{mol})$ |
| 17.93 | 480.2 |  |  |  |  | A | 11.92 |
| 20.06 | 559.1 |  |  |  |  | B | 4994 |

2. 

| Robbins et al. 1993 |  | Perlinger et al. 1993 |  | Dewulf et al. 1995 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| static headspace-GC |  | equilibrium headspace-GC |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 25 | 788 | 10 | 306 | 2 | 180 |
| 30 | 1034 | 15 | 428 | 6 | 194 |
| 40 | 1662 | 20 | 583 | 10 | 257 |
|  |  | 25 | 660 | 18.2 | 497 |
| eq. 4 | $\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ | 30 | 1044 | 25 | 669 |
| A | 7.14 |  |  |  |  |
| B | 3689 |  |  | eq 1 | $\mathrm{K}_{\text {AW }}$ |
|  |  |  |  | A | 14.001 |
|  |  |  |  | B | 4567 |



FIGURE 3.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for ethylbenzene.

### 3.1.1.4 o-Xylene



Common Name: o-Xylene
Synonym: 1,2-dimethylbenzene, $o$-xylol, 2-methyltoluene
Chemical Name: o-xylene
CAS Registry No: 95-47-6
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{10}, \mathrm{C}_{6} \mathrm{H}_{4}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 106.165
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-25.2 (Weast 1982-83; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 144.5 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8802 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $120.6 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 43.434, $36.82 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 13.6 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$
55.23 (Yalkowsky \& Valvani 1980)
54.9, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated ${ }^{*}$, are compiled at the end of this section):

| 204 | (shake flask-UV, Andrews \& Keefer 1949) |
| :--- | :--- |
| 175 | (shake flask-GC, McAuliffe 1963) |
| 175 | (shake flask-GC, McAuliffe 1966) |
| 176 | (shake flask-GC, Hermann 1972) |
| $213^{*}$ | (shake flask-GC, Polak \& Lu 1973) |
| 170.5 | (shake flask-GC, Sutton \& Calder 1975) |
| 167 | (shake flask-GC, Price 1976) |
| 167 | (shake flask-GC, Krzyzanowska \& Szeliga 1978) |
| $240^{*}$ | (20 ${ }^{\circ} \mathrm{C}$, shake flask-UV, Ben-Naim \& Wiff 1979) |
| $179^{*}$ | (vapor saturation-UV spec., measured range 15-45 ${ }^{\circ} \mathrm{C}$, Sanemasa et al. 1982) |
| 221 | (generator column-HPLC/UV, Tewari et al. 1982c) |
| 221 | (generator column-HPLC/UV, Wasik et al. 1983) |
| 176 | (shake flask-purge and trap-GC, Coutant \& Keigley 1988) |
| $173^{*}$ | (IUPAC recommended value, temp range 0-45 ${ }^{\circ} \mathrm{C}$, Shaw 1989b) |

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
146.7* $\quad\left(0.60^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -17 to $0.60^{\circ} \mathrm{C}$, Linder 1931)

767* ( $20^{\circ} \mathrm{C}, \mathrm{Hg}$ manometer, Kassel 1936)
$\log (\mathrm{P} / \mathrm{mmHg})=-2830.0 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+22.7480$; temp range $0-80^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)
987* ( $30^{\circ} \mathrm{C}, \mathrm{Hg}$ manometer, measured range $10-50^{\circ} \mathrm{C}$, Rintelen et al. 1937)
$\log (\mathrm{P} / \mathrm{mmHg})=-2908.07 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+22.95279$; temp range $4-75^{\circ} \mathrm{C}$ (vapor pressure eq. from manometer measurements, Stuckey \& Saylor 1940)
880* (Hg manometer measurements, Pitzer \& Scott 1943)
$\log (\mathrm{P} / \mathrm{mmHg})=-3327.16 /(\mathrm{T} / \mathrm{K})-8.0 \log (\mathrm{~T} / \mathrm{K})+31.7771$; temp range $0-60^{\circ} \mathrm{C}$ (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer \& Scott 1943)
$6354^{*} \quad\left(63.460^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $63.460-145.367^{\circ} \mathrm{C}$, Willingham et al. 1945)
$6401^{*} \quad\left(63.608^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $63.608-145.400^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99937-1474.969 /\left(213.714+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $63.5-145.4^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
266.6* (20.2 ${ }^{\circ} \mathrm{C}$, summary of literature data, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99891-1474.679 /\left(213.686+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $63.6-145.4^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
892 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99891-1474.679 /\left(213.686+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $50-200^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1333* $\quad\left(32.155^{\circ} \mathrm{C}\right.$, compiled data, temp range $32.155-172.095^{\circ} \mathrm{C}$, Bond \& Thodos 1960)
108000* $\quad\left(146.85^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $146.85-346.85^{\circ} \mathrm{C}$, Ambrose et al. 1967)
882* (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99891-1474.679 /\left(213.686+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32.14-172.07^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9998.5 /(\mathrm{T} / \mathrm{K})]+8.147551$; temp range -3.8 to $144.4^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{atm})=(1-417.496 / \mathrm{T}) \times 10^{\wedge}\left(0.855257-6.48662 \times 10^{4} \cdot \mathrm{~T}+5.53883 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range: 253.2-631.64 K (Cox vapor pressure eq., Chao et al. 1983)

882, 885 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.12699-1476.753 /\left(213.911+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $63.46-145.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.9422-1387.336 /\left(206.409+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $0-50^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Pitzer \& Scott 1943, Boublik et al. 1984)
882 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99891-1474.679 /\left(213.69+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32-172^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
$880 \quad$ (Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.13072-1479.82 /\left(214.315+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
885 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.13132-1480.155 /(-58.804+\mathrm{T} / \mathrm{K})$; temp range $333-419 \mathrm{~K}$ (liquid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.15921-1502.949 /(-55.725+\mathrm{T} / \mathrm{K})$; temp range $416-473 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.46119-1772.963 /(-18.84+\mathrm{T} / \mathrm{K})$; temp range $471-571 \mathrm{~K}$ (liquid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.91427-3735.582 /(229.953+\mathrm{T} / \mathrm{K})$; temp range $567-630 \mathrm{~K}$ (liquid, Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=37.2413-3.4573 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.126 \cdot \log (\mathrm{~T} / \mathrm{K})+9.0676 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+2.6123 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 248-630 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
542, 506 (calculated as $1 / \mathrm{K}_{\mathrm{AW}}$, calculated-bond contribution, Hine \& Mookerjee 1975)
647 (vapor liquid equilibrium-concentration ratio, Leighton \& Calo 1981)
526* (vapor-liquid equilibrium, Sanemasa et al. 1982)
$594 \quad\left(20^{\circ} \mathrm{C}\right.$, EPICS-GC, Yurteri et al. 1987)
493* (EPICS-GC/FID, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=5.541-3220 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
424 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
592 (concentration ratio, Anderson 1992)
1067* ( $40^{\circ} \mathrm{C}$, equilibrium headspace-GC, Kolb et al. 1992)
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=-7.61+2647 /(\mathrm{T} / \mathrm{K})$, temp range $40-80^{\circ} \mathrm{C}$ (equilibrium headspace-GC measurements, Kolb et al. 1992)

485 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
506* (static headspace-GC, Robbins et al. 1993)
372 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
429* (EPICS-GC/FID, measured range $2-25^{\circ} \mathrm{C}$, Dewulf et al. 1995)
189, $496\left(6.0,25^{\circ} \mathrm{C}\right.$, EPICS-GC/FID, natural seawater with salinity of $35 \%$ o Dewulf et al. 1995)
$\ln \mathrm{K}_{\mathrm{AW}}=-4232 /(\mathrm{T} / \mathrm{K})+0.01115 \cdot \mathrm{Z}+12.400$; with Z salinity $0-35.5 \%$, temp range: $2-35^{\circ} \mathrm{C}(\mathrm{EPICS}-\mathrm{GC} / \mathrm{FID}$, Dewulf et al. 1995)
$412\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
731 (vapor-liquid equilibrium-GC, Turner et al. 1996)
464.4 (exponential saturator EXPSAT technique, Dohnal \& Hovorka 1999)
$390 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=5.064-1719 /(\mathrm{T} / \mathrm{K})($ van't Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ at $25^{\circ} \mathrm{C}$ :
3.15 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
2.73 (shake flask-LSC, Banerjee et al. 1980)
3.19 (HPLC-k' correlation, Hammers et al. 1982)
3.13 (generator column-HPLC/UV, Tewari et al. 1982b,c)
3.13 (generator column-HPLC/UV, Wasik et al. 1983)
3.13, $3.14,3.14,3.06,3.16,3.42 \quad$ (quoted exptl.; calculated $-\pi$ const., f const., MW, MCI $\chi$, TSA, Doucette \& Andren 1988)
3.25, 3.35 (RP-HPLC-k' capacity factor correlations, Sherblom \& Eganhouse 1988)
3.12 (recommended, Sangster 1989)
3.18 (normal phase HPLC- $\mathrm{k}^{\prime}$ correlation, Govers \& Evers 1992)
3.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
3.80* $\quad\left(30.3^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range $30.3-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997) 3.72 (calculated-measured $\gamma^{\infty}$ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
1.33 (eels, Ogata \& Miyake 1978)
0.79 (clams, Nunes \& Benville 1979)
1.15 (goldfish, Ogata et al. 1984)
2.34 (S. capricornutum, Herman et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ :
1.68-1.83 (Nathwani \& Philip 1977)
2.35 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
2.73 (HPLC-k' correlation, cyanopropyl column, Hodson \& Williams 1988)
2.37, 2.40 (RP-HPLC-k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
3.13 (average of 5 soils, sorption isotherms by batch equilibrium method, Xing et al. 1994)
2.36, 2.65, 2.65 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al. 1995)
2.45, 2.45 (RP-HPLC- $\mathrm{k}^{\prime}$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
$2.40,2.70,2.58,2.68,2.73,2.69,2.68 \quad\left(2.3,3.8,6.2,8.0,13.5,18.6,25^{\circ} \mathrm{C}\right.$, natural sediment from River Leie, organic carbon $f_{\text {OC }}=4.12 \%$, EPICS-GC/FID, Dewulf et al. 1999)

Environmental Fate Rate Constants, k , or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $\mathrm{t}_{1 / 2}=5.61 \mathrm{~h}$ from water depth of 1 m (Mackay \& Leinonen 1975; Haque et al. 1980);
$t_{1 / 2} \sim 3.2 \mathrm{~h}$ of evaporation from water of 1 m depth with wind speed of $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{s}$ (Lyman et al. 1982);
$t_{1 / 2} \sim 31-125 \mathrm{~h}$ of evaporation from a typical river or pond (Howard 1990).
Photolysis: $\mathrm{k}=7.46 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with HO - in the gas (Dilling et al. 1988).
Oxidation: rate constant k ; for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated $*$, see reference:
$\mathrm{k}_{\mathrm{OH}}=(7.7 \pm 2.3) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(1.05 \pm 0.11) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(15.3 \pm 1.5) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(1.74 \pm 0.18) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=8.4 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-24 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(14.3 \pm 1.5) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured over temp range 296-473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)
$\mathrm{k}_{\mathrm{OH}}=(12.9,13.0,12.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=13.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{m}^{-1} \mathrm{~s}^{-1}$ and residence time of 0.8 d , loss of $71.3 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{\mathrm{O} 3}<0.01 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ with a calculated lifetime $\tau>2300 \mathrm{~d}$, and a calculated lifetime of 0.8 d due to reaction with OH radical at room temp. (Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{O} 3}=950 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Lyman et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=(5.9-12) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.47-1.0 \mathrm{~d}$ (Mill 1982)
$\mathrm{k}=(90 \pm 20) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water at $\mathrm{pH} 1.7-5.0$ and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{NO} 3}=1.1 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=13.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=4.4-44 \mathrm{~h}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=12.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=12.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $24.2^{\circ} \mathrm{C}$, with a calculated atmospheric lifetime of 0.93 d (Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.14.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship] Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}=1.47 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=3.74 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{O} 3}<0.01 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=1.47 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=3.7 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ at room temp. (Atkinson \& Aschmann 1988)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=1.37 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ independent over $296-320 \mathrm{~K}$ (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=13.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.92 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=14.75 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.51 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ exptl $)=13.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok \& Atkinson 1995)
Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).
Biodegradation:
$100 \%$ biodegraded after 192 h at $13^{\circ} \mathrm{C}$ with an initial conen of $1.62 \times 10^{-6} \mathrm{~L} / \mathrm{L}$ (Jamison et al. 1976);
$\mathrm{t}_{1 / 2}$ (aq. Aerobic) $=168-672 \mathrm{~h}$, estimated based on aqueous screening test data (Bridie et al. 1979; Howard et al. 1991) and soil column study simulating an aerobic river/ground-water infiltration system (Kuhn et al. 1985; Howard et al. 1991)
$t_{1 / 2}($ aq. anaerobic $)=4320-8640 \mathrm{~h}$, estimated based on acclimated grab sample data for anaerobic soil from a groundwater aquifer receiving landfill leachate (Wilson et al. 1986) and a soil column study simulating an anaerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)
$\mathrm{k}=0.06 \mathrm{yr}^{-1}$ with $\mathrm{t}_{1 / 2}=32 \mathrm{~d}$ (Olsen \& Davis 1990)
$\mathrm{t}_{1 / 2}($ aerobic $)=7 \mathrm{~d}, \mathrm{t}_{1 / 2}($ anaerobic $)=180 \mathrm{~d}$ in natural waters $($ Capel \& Larson 1995)
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: $t_{1 / 2}=0.24-2.4 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976);
residence time of 0.8 d , loss of $71.3 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
calculated lifetimes $\tau>2300 \mathrm{~d}$ and 0.8 d due to reactions with $\mathrm{O}_{3}$ and OH radical respectively at room temp. (Atkinson et al. 1982);
$\mathrm{t}_{1 / 2}=4.4-44 \mathrm{~h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);
summer daylight lifetime $\tau=10 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991);
calculated lifetime $\tau=0.93$ d due to reaction with OH radical (Edney et al. 1986).
Surface Water: photooxidation $\mathrm{t}_{1 / 2}=3.9 \times 10^{5}-2.7 \times 10^{8} \mathrm{~h}$ in water, based on estimated rate data for alkoxyl radical in aqueous solution (Hendry et al. 1974);
$\mathrm{t}_{1 / 2}=5.18 \mathrm{~h}$, based on evaporative loss at $25^{\circ} \mathrm{C}$ and 1 m depth of water (Mackay \& Leinonen 1975; Haque et al. 1980);
$t_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);
$t_{1 / 2}=1-5 \mathrm{~d}$, volatilization to be the dominant removal process (Howard 1990).
$\mathrm{t}_{1 / 2}($ aerobic $)=7 \mathrm{~d}, \mathrm{t}_{1 / 2}($ anaerobic $)=180 \mathrm{~d}$ in natural waters $($ Capel \& Larson 1995)
Ground water: $t_{1 / 2}=336-8640 \mathrm{~h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Wilson et al. 1986; Howard et al. 1991);
$\mathrm{t}_{1 / 2} \sim 0.3 \mathrm{yr}$ from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).
Soil: $t_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).
Biota: $\mathrm{t}_{1 / 2}=2 \mathrm{~d}$ to eliminate from eels in seawater (Ogata \& Miyake 1978).

TABLE 3.1.1.4.1
Reported aqueous solubilities of $o$-xylene at various temperatures

| Polak \& Lu 1973 |  | Ben-Naim \& Wiff 1979 |  | Sanemasa 1982 |  | Shaw 1989b (IUPAC) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-GC |  | shake flask-UV |  | vapor saturation-UV |  | recommended values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 0 | 142 | 10 | 212.4 | 15 | 168 | 0 | 140 |
| 25 | 213 | 20 | 240 | 25 | 179 | 15 | 170 |
|  |  |  |  | 35 | 198 | 25 | 173 |
|  |  |  |  | 45 | 214 | 35 | 200 |
|  |  |  |  |  |  | 45 | 210 |



FIGURE 3.1.1.4.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $o$-xylene.

TABLE 3.1.1.4.2
Reported vapor pressures of o-xylene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \cdot \mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}$
1.

2.

| Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  | Bond \& Thodos 1960 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | summary of literature data |  | ebulliometry |  | compiled data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 63.460 | 6354 | -3.80 | 133.3 | 63.608 | 6401 | 32.155 | 1333 |
| 67.746 | 7654 | 20.2 | 266.6 | 67.852 | 7693 | 63.48 | 6354 |
| 71.481 | 8963 | 32.1 | 1333 | 71.548 | 8991 | 74.87 | 10303 |
| 74.857 | 10303 | 45.1 | 2666 | 74.916 | 10331 | 112.46 | 39997 |
| 77.993 | 11699 | 59.5 | 5333 | 78.048 | 11722 | 141.35 | 93326 |
| 82.242 | 13819 | 68,8 | 7999 | 82.285 | 13843 | 172.095 | 199984 |
| 87.081 | 16621 | 81.3 | 13332 | 87.101 | 16635 |  |  |
| 91.987 | 19924 | 100.2 | 26664 | 92.015 | 19945 | eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ |
| 96.541 | 23450 | 121.7 | 53329 | 96.568 | 23475 | A | 25.82849 |
| 102.632 | 28954 | 144.4 | 101325 | 102.657 | 28979 | B | 3040.72 |
| 108.227 | 34897 |  |  | 198.250 | 34926 | C | 5.94175 |
| 114.965 | 43322 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -25.2 | 114.988 | 43362 | D | 2.61456 |
| 121.909 | 53654 |  |  | 121.935 | 53700 |  |  |
| 129.318 | 66756 |  |  | 129.333 | 66797 | bp/ ${ }^{\circ} \mathrm{C}$ | 144.426 |
| 137.346 | 83717 |  |  | 137.356 | 83750 |  |  |
| 143.007 | 97604 |  |  | 143.619 | 97647 |  |  |
| 143.614 | 99200 |  |  | 143.626 | 99236 |  |  |
| 144.176 | 100692 |  |  | 144.190 | 87395 |  |  |
| 144.809 | 102385 |  |  | 144.832 | 90465 |  |  |

TABLE 3.1.1.4.2 (Continued)

| Willingham et al. 1945 |  | Stull 1947 |  | Forziati et al. 1949 |  | Bond \& Thodos 1960 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | summary of literature data |  | ebulliometry |  | compiled data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 145.367 | 103905 |  |  | 145.400 | 104000 |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
| A | 6.99937 |  |  | A | 6.99891 |  |  |
| B | 1474.967 |  |  | B | 1474.679 |  |  |
| C | 144.414 |  |  | C | 213.686 |  |  |
| bp/ ${ }^{\circ} \mathrm{C}$ | 144.414 |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 144.411 |  |  |

3. 

Ambrose et al. 1967
Zwolinski \& Wilhoit 1971

| ebulliometry |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 146.85 | 108000 | 32.14 | 1333 | 145.395 | 103991 |
| 166.85 | 177200 | 45.13 | 2666 | 146.359 | 106658 |
| 186.85 | 276700 | 53.38 | 4000 | 150.912 | 119990 |
| 206.85 | 413900 | 59.56 | 5333 | 155.08 | 13322 |
| 226.85 | 598300 | 64.558 | 6666 | 162.53 | 159987 |
| 246.85 | 839100 | 68.778 | 7999 | 172.07 | 199984 |
| 266.85 | 1146500 | 75.704 | 10666 | 25.0 | 879.9 |
| 286.85 | 1532100 | 81.314 | 13332 |  |  |
| 306.85 | 2009000 | 92.085 | 19998 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 326.85 | 2592500 | 100.217 | 26664 | A | 6.99891 |
| 346.85 | 3304100 | 106.829 | 33331 | B | 1474.679 |
|  |  | 112.441 | 39997 | C | 213.686 |
| eq. 5 | P/bar | 121.708 | 53329 |  |  |
| A | 20.79970 | 129.267 | 66661 | bp/ ${ }^{\circ} \mathrm{C}$ | 144.411 |
| B | 2921.11 | 135.700 | 79993 |  |  |
| C | 5.26888 | 141.332 | 93326 | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |  |
| D | 1672 | 142.380 | 95991 | at $25^{\circ} \mathrm{C}$ | 43.43 |
| $1 \mathrm{bar}=1 \times 10^{5} \mathrm{~Pa}$ |  | 143.407 | 98659 | at bp | 36.82 |
|  |  | 144.411 | 101325 |  |  |



FIGURE 3.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for o-xylene.

## TABLE 3.1.1.4.3

Reported Henry's law constants of $o$-xylene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln [\mathrm{H} /(\mathrm{Pa} \mathrm{m}$
$3 / \mathrm{mol})]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B}(\mathrm{T} / \mathrm{K})+\mathrm{C}(\mathrm{T} / \mathrm{K})^{2}$
(1) $\quad \log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(2) $\quad \log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(3)
(4) $\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

| Sanemasa et al. 1982 |  | Ashworth et al. 1988 |  | Kolb et al. 1992 |  | Robbins et al. 1993 |  | Dewulf et al. 1995 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| vapor-liquid equilibrium |  | EPICS-GC |  | headspace-GC |  | static headspace-GC |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | $\begin{gathered} \mathrm{H} /(\mathrm{Pa} \\ \left.\mathbf{m}^{3} / \mathrm{mol}\right) \end{gathered}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\begin{gathered} \mathrm{H} /(\mathrm{Pa} \\ \left.\mathrm{m}^{3} / \mathrm{mol}\right) \end{gathered}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\begin{gathered} \mathrm{H} /(\mathrm{Pa} \\ \left.\mathbf{m}^{3} / \mathrm{mol}\right) \end{gathered}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\begin{gathered} \mathrm{H} /(\mathrm{Pa} \\ \left.\mathbf{m}^{3} / \mathrm{mol}\right) \end{gathered}$ |
| 15 | 299 | 10 | 289 | 40 | 1067 | 25 | 506 | 2 | 133 |
| 25 | 526 | 15 | 366 | 60 | 2114 | 30 | 637 | 6 | 118 |
| 35 | 844 | 20 | 480 | 70 | 2825 | 40 | 1104 | 10 | 155 |
| 45 | 1323 | 25 | 493 | 80 | 2966 | 45 | 1074 | 18 | 325 |
|  |  | 30 | 634 |  |  | 50 | 1175 | 25 | 429 |
|  |  | eq. 4 a |  | eq. 2 | $\mathrm{K}_{\text {AW }}$ | eq. 4 |  | eq 1 | $\mathrm{K}_{\text {AW }}$ |
|  |  | $\mathrm{H} /(\mathrm{atm} \mathrm{m} 3 / \mathrm{mol})$ |  | A | 761 |  | Pa m ${ }^{3} / \mathrm{mol}$ ) | A | 12.4 |
|  |  | A | 5.541 | B | 2647/R | A | 17.67818 | B | 4243 |
|  |  | B | 3220 |  |  | B | 3397.97 |  |  |



FIGURE 3.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for o-xylene.

TABLE 3.1.1.4.4
Reported octanol-air partition coefficients of $o$ xylene at various temperatures

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|  | GC det'd activity coefficient |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\boldsymbol{\operatorname { l o g }} \mathbf{K}_{\text {OA }}$ |
| 20.29 | - |
| 30.3 | 3.80 |
| 40.4 | 3.59 |
| 50.28 | 3.38 |

### 3.1.1.5 m-Xylene



Common Name: $m$-Xylene
Synonym: 1,3-dimethylbenzene, $m$-xylol, 3-methyltoluene
Chemical Name: $m$-xylene
CAS Registry No: 108-38-3
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{10}, \mathrm{C}_{6} \mathrm{H}_{4}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 106.165
Melting Point ( ${ }^{\circ} \mathrm{C}$ ) -47.8 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 139.12 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8842 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$120.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 42.656, $36.36 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 11.57 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 51.88 (Yalkowsky \& Valvani 1980) 51.4, 45.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$, or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
173 (shake flask-UV, Andrews \& Keefer 1949)
196* (shake flask-UV, measured range $0.4-39.6^{\circ} \mathrm{C}$, Bohon \& Claussen 1951)
157 (shake flask-GC, Hermann 1972)
162* (shake flask-GC, Polak \& Lu 1973)
206 (shake flask-UV, Vesala 1974)
146 (shake flask-GC, Sutton \& Calder 1975)
160* (synthetic method-GC, measured range $20-70^{\circ} \mathrm{C}$, Chernoglazova \& Simulin 1976)
134 (shake flask-GC, Price 1976)
134 (shake flask-GC, Krzyzanowska \& Szeliga 1978)
162* (vapor saturation-UV spec., measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
159 (generator column-HPLC/UV, Tewari et al. 1982c)
160 (generator column-HPLC/UV, Wasik et al. 1983)
160* (IUPAC recommended value, temp range $0-70^{\circ} \mathrm{C}$, Shaw 1989b)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$1812.7^{*} \quad\left(-2.80^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -8.40 to $-2.80^{\circ} \mathrm{C}$, Linder 1931)
833* ( $20^{\circ} \mathrm{C}, \mathrm{Hg}$ manometer, Kassel 1936)
$\log (\mathrm{P} / \mathrm{mmHg})=-2876.3 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+22.9425$; temp range $0-80^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)
1213* $\left(30^{\circ} \mathrm{C}, \mathrm{Hg}\right.$ manometer, measured range $10-50^{\circ} \mathrm{C}$, Rintelen et al. 1937)
$\log (\mathrm{P} / \mathrm{mmHg})=-2870.38 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+22.92341$; temp range $4-75^{\circ} \mathrm{C}$ (vapor pressure eq. from manometer measurements, Stuckey \& Saylor 1940)
1113* (Hg manometer, measured range $0-60^{\circ} \mathrm{C}$, Pitzer \& Scott 1943)
$\log (\mathrm{P} / \mathrm{mmHg})=-2871.66 /(\mathrm{T} / \mathrm{K})-5.0 \log (\mathrm{~T} / \mathrm{K})+22.9270$; temp range $0-60^{\circ} \mathrm{C}$ (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer \& Scott 1943)
$6355^{*} \quad\left(59.203^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $59.203-140.041^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00343-1458.214 /\left(214.609+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $59.2-140.0^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
$266.6^{*} \quad\left(16.8^{\circ} \mathrm{C}\right.$, summary of literature data, temp range -6.9 to $139.1^{\circ} \mathrm{C}$, Stull 1947)
$6400^{*} \quad\left(59.335^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $59.335-140.078^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=8.00849-1461.925 /\left(215.073+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $59.3-140.1^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
1115 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00908-1462.266 /\left(215.105+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $45-195^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
124200* $\quad\left(146.85^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $146.85-316.85^{\circ} \mathrm{C}$, Ambrose et al. 1967)
1100* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00908-1462.266 /\left(215.105+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $28.24-166.39^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9904.2 /(\mathrm{T} / \mathrm{K})]+8.167049$; temp range -6.9 to $139.1^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{atm})=(1-3412.335 / \mathrm{T}) \times 10^{\wedge}\left(0.859841-6.73249 \times 10^{4} \cdot \mathrm{~T}+5.87438 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 243.2-619.2 K (Cox vapor pressure eq., Chao et al. 1983)

1104, 1142 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.13232-1460.805 /\left(214.895+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $59.2-140.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.4729-1641.628 /\left(230.899+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range: $0-60^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Pitzer \& Scott 1943, Boublik et al. 1984)
1106 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00908-1462.266 /\left(215.11+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $28-166^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
1100 (selected lit. value., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.13785-1465.39 /\left(215.512+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
1110 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.14083-1457.244 /(-57.442+\mathrm{T} / \mathrm{K})$; temp range $331-414 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.76037-1292.22 /(-72.052+\mathrm{T} / \mathrm{K})$; temp range $267-301 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.17035-1490.184 /(-54.184+\mathrm{T} / \mathrm{K})$; temp range $412-462 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.42535-1710.901 /(-24.591+\mathrm{T} / \mathrm{K})$; temp range $461-554 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.59221-3163.74 /(165.278+\mathrm{T} / \mathrm{K})$; temp range $550-617 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=34.6803-3.2981 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.2570 \cdot \log (\mathrm{~T} / \mathrm{K})-4.3563 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+2.4103 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $226-617 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$, are compiled at the end of this section):
731* (vapor-liquid equilibrium, Sanemasa et al. 1982)
754* (EPICS-GC/FID, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=6.280-3337 /(\mathrm{T} / \mathrm{K})$; temp range: $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
675 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
665 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
739* (static headspace-GC, same as p-xylene, Robbins et al. 1993)
615* (EPICS-GC/FID, measured range $2-25^{\circ} \mathrm{C}$, Dewulf et al. 1995)

297, $771 \quad\left(6.0,25^{\circ} \mathrm{C}\right.$, EPICS-GC/FID, natural seawater with salinity of 35\%, Dewulf et al. 1995) $\ln \mathrm{K}_{\mathrm{AW}}=-4026 /(\mathrm{T} / \mathrm{K})+0.00846 \cdot \mathrm{Z}+12.123$; with Z salinity $0-35.5 \%$, temp range: $2-35^{\circ} \mathrm{C}$ (EPICS-GC/FID, Dewulf et al. 1995)
$590 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
658.5 (exponential saturator EXPSAT technique, Dohnal \& Hovorka 1999)
$561 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=5.204-1713 /(\mathrm{T} / \mathrm{K})($ van't Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ at $25^{\circ} \mathrm{C}$ :
3.20 (Hansch et al. 1968; Leo et al. 1971; Hansch \& Leo 1979; Hansch \& Leo 1985)
3.18 (generator column-HPLC/UV, Wasik et al. 1981)
3.29 (HPLC-k' correlation, Hammers et al. 1982)
3.13 (generator column-HPLC/UV, Tewari et al. 1982b,c)
3.20 (generator column-HPLC/UV, Wasik et al. 1983)
3.28 (HPLC-RV retention volume correlation, Garst \& Wilson 1984)
3.37 (HPLC-k' correlation, Haky \& Young 1984)
3.33, 3.45 (RP-HPLC-k' capacity factor correlations, Sherblom \& Eganhouse 1988)
3.20 (recommended, Sangster 1989, 1993)
3.31 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
3.20 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:
3.69* $\quad\left(30.3^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range $30.3-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997)
3.79 (calculated-measured $\gamma^{\infty}$ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:

| 1.37 | (eels, Ogata \& Miyake 1978) |
| :--- | :--- |
| 0.78 | (clams, Nunes \& Benville 1979) |
| 1.17 | (goldfish, Ogata et al. 1984) |
| 2.40 | (S. capricornutum, Herman et al. 1991) |

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ :
2.11, 2.48, 2.20 (forest soil pH 5.6 , forest soil pH 4.2 , agricultural soil pH 7.4 , Seip et al. 1986)
2.37, 2.40 (RP-HPLC-k' correlation, Szabo et al. 1990a,b)
2.62, 2.63 (RP-HPLC-k' correlation including MCI related to non-dispersive intermolecular interac-
tions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.06, 2.33 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%, \mathrm{OC} \geq 0.5 \%$, average, Delle Site 2001)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1 / 2}$ :
Volatilization: $t_{1 / 2} \sim 3.1 \mathrm{~h}$ for evaporation from water of 1 m depth with wind speed of $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{s}$ (Lyman et al. 1982);
$t_{1 / 2} \sim 27-135 \mathrm{~h}$ for evaporation from a typical river or pond (Howard 1990).
Photolysis:
Oxidation: rate constant k ; for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated ${ }^{*}$, see reference:
photooxidation $t_{1 / 2}=4.8 \times 10^{6}-2.4 \times 10^{8} \mathrm{~h}$ in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974)
$\mathrm{k}_{\mathrm{OH}}=(14 \pm 1) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.83 \mathrm{~h} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(2.12 \pm 0.21) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=1.4 \times 10^{10} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with an initial concn of $2.0 \times 10^{-10} \mathrm{~mol} \mathrm{~L}^{-1}$ at 300 K (Doyle et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=(23.6 \pm 2.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(3.52 \pm 0.35) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=(12.9 \pm 2.6) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=14.1 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(24.0 \pm 2.5) \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured over temp range 296-473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)
$\mathrm{k}_{\mathrm{OH}}=(15.6-21.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysisresonance fluorescence, Ravishanakara et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=23.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and residence time of 0.5 d , loss of $86.5 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{\mathrm{O} 3}<0.005 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated lifetime $\tau>1150 \mathrm{~d}$ and a lifetime $\tau=0.5 \mathrm{~d}$ due to reaction with OH radical at room temp. (Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{O} 3}=780 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone at 300 K (Lyman et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=(5.9-12) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.47-1.0 \mathrm{~d}$ for xylenes (Mill 1982)
$\mathrm{k}=(94 \pm 20) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water using $1 \mathrm{mM} t-\mathrm{BuOH}$ as scavenger at pH 2.0 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{NO} 3}=7.1 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=23.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=2.6-26 \mathrm{~h}$ in air (Atkinson 1985; Howard et al. 1991)
$\mathrm{k}_{\mathrm{OH}}=22.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=22.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} 23.5^{\circ} \mathrm{C}$, with a calculated atmospheric lifetime $\tau=0.51 \mathrm{~d}$ (Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=14 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}\left(\mathrm{obs}\right.$.) $=24.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{NO} 3}=2.49 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=2.45 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=2.36 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=1.45 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=17.47 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
$\mathrm{k}_{\mathrm{OH}}=(1.81 \pm 0.40) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $(2.03 \pm 0.10) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Phousongphouang \& Arey 2002)
Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).
Biodegradation:
$100 \%$ biodegraded after 192 h at $13^{\circ} \mathrm{C}$ with an initial concn of $3.28 \times 10^{-6} \mathrm{~L} / \mathrm{L}$ (Jamison et al. 1976)
$t_{1 / 2}($ aq. aerobic $)=168-672 \mathrm{~h}$, based on aqueous screening test data (Bridie et al. 1979; Howard et al. 1991) and soil column study simulating an aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=672-2688 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)
$\mathrm{t}_{1 / 2}=0.03 \mathrm{~d}$ (Olsen \& Davis 1990)
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.83 \mathrm{~h}$, based on rate of disappearance for the reaction with OH radical in ambient LA basin air at 300
K (Doyle et al. 1975);
photodecomposition $t_{1 / 2}=2.9 \mathrm{~h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976);
estimated lifetime $\tau=1.5 \mathrm{~h}$ under photochemical smog conditions in S.E. England (Brice \& Derwent 1978) and (Perry et al. 1977);
residence time of 0.5 d , loss of $86.5 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
calculated lifetimes $\tau>1150 \mathrm{~d}$ and 0.5 d due to reactions with $\mathrm{O}_{3}$ and OH radical, respectively, at room temp. (Atkinson et al. 1982);
$t_{1 / 2}=2.6-26 \mathrm{~h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);
calculated atmospheric lifetime $\tau=0.51$ d due to reaction with OH radical (Edney et al. 1986);
summer daylight lifetime $\tau=5.9 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991);
calculated lifetimes of $5.9 \mathrm{~h}, 200 \mathrm{~d}$ and $>4.5 \mathrm{yr}$ for reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$, respectively (Atkinson 2000).
Surface Water: $t_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979;
Kuhn et al. 1985; Howard et al. 1991);
volatilization appears to be dominant removal process with $t_{1 / 2}=1-5.5 \mathrm{~d}$ (Howard 1990).

Ground water: $\mathrm{t}_{1 / 2}=336-8640 \mathrm{~h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);
$t_{1 / 2} \sim 0.3 \mathrm{yr}$ from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981); abiotic hydrolysis or dehydro-halogenation $t_{1 / 2}=377$ months (Olsen \& Davis 1990).
Soil: $\mathrm{t}_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).
Biota: $t_{1 / 2}=2 \mathrm{~d}$, half-life to eliminate from eels in seawater (Ogata \& Miyake 1978).

TABLE 3.1.1.5.1
Reported aqueous solubilities of $\boldsymbol{m}$-xylene at various temperatures

| Bohon \& Claussen 1951 |  | Polak \& Lu 1973 |  | Sanemasa et al. 1982 |  | Shaw 1989b (IUPAC) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-GC |  | vapor saturation-UV |  | recommended values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0.4 | 209 | 0 | 196 | 15 | 158 | 0 | 203 |
| 5.2 | 201 | 25 | 162 | 25 | 162 | 10 | 200 |
| 14.9 | 192 |  |  | 35 | 168 | 20 | 170 |
| 21 | 196 |  |  | 45 | 186 | 25 | 160 |
| 25 | 196 |  |  |  |  | 30 | 180 |
| 25.6 | 196 |  |  |  |  | 40 | 220 |
| 30.3 | 198 |  |  | $\Delta \mathrm{H}_{\text {s }}$ | ) $=2.60$ | 50 | 230 |
| 34.9 | 203 |  |  |  |  | 60 | 320 |
| 39.6 | 218 |  |  |  |  | 70 | 350 |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  | Chernoglazova \& Simulin 1976 |  |  |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=2.9$ |  |
| $25^{\circ} \mathrm{C}$ | 2.8 | synthetic method-GC |  |  |  | (calc from Van't Hoff eq.) |  |
| $2^{\circ} \mathrm{C}$ | -5.506 | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S / g} \cdot \mathrm{m}^{-3}$ |  |  |  |  |
| $7{ }^{\circ} \mathrm{C}$ | -3.828 |  |  |  |  |  |  |
| $12^{\circ} \mathrm{C}$ | -1.59 | 20 | 160 |  |  |  |  |
| $17^{\circ} \mathrm{C}$ | 0 | 40 | 220 |  |  |  |  |
| $22^{\circ} \mathrm{C}$ | 1.22 | 70 | 380 |  |  |  |  |
| $27^{\circ} \mathrm{C}$ | 1.99 |  |  |  |  |  |  |
| $32^{\circ} \mathrm{C}$ | 3.92 | $\begin{gathered} \Delta \mathrm{H}_{\text {sol }}\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=11.9 \\ \text { between } 127-239^{\circ} \mathrm{C} \end{gathered}$ |  |  |  |  |  |
| $37^{\circ} \mathrm{C}$ | 8.87 |  |  |  |  |  |  |



FIGURE 3.1.1.5.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $m$-xylene.

TABLE 3.1.1.5.2
Reported vapor pressures of $m$-xylene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D}(\mathrm{T} / \mathrm{K})^{2}$
1.

| Kassel 1936 |  | Rintelen et al. 1937 |  | Pitzer \& Scott 1943 |  | Willingham et al. 1945 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer |  | mercury manometer |  | mercury manometer |  | ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
| 0 | 228 | 10 | 293 | 0 | 233 | 59.203 | 6355 |
| 10 | 433 | 30 | 1213 | 12.5 | 520 | 68.436 | 7654 |
| 20 | 833 | 50 | 3906 | 25 | 1113 | 67.123 | 8963 |
| 30 | 1480 |  |  | 37.7 | 2220 | 70.458 | 9272 |
| 40 | 2533 |  |  | 50 | 4160 | 73.588 | 11698 |
| 50 | 4173 | bp/ ${ }^{\circ} \mathrm{C}$ | 138.99 | 60 | 6600 | 77.747 | 13819 |
| 60 | 6626 |  | 139.15 |  |  | 82.522 | 16621 |
| 70 | 10212 |  |  |  |  | 87.367 | 19924 |
| 80 | 15280 |  |  |  |  | 91.86 | 23450 |
|  |  |  |  | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 97.87 | 28954 |
| eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | A | 22.927 | 103.396 | 34897 |
| A | 22.9425 |  |  | B | 2871.66 | 110.041 | 43322 |
| B | 2876.3 |  |  | C | 5 | 116.896 | 53654 |
| C | 5 |  |  |  |  | 124.205 | 66755 |
|  |  |  |  | $\Delta \mathrm{H}_{V}$ | $\mathrm{mol}^{-1}$ ) | 132.128 | 83717 |
|  |  |  |  | 298 K | 42.51 | 137.713 | 97604 |
|  |  |  |  |  |  | 138.314 | 99200 |
|  | 1931 | Stuckey | ylor 1940 |  |  | 138.869 | 100692 |
| mercury manometer |  | mercury manometer |  |  |  | 139.493 | 102385 |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |  |  | 140.041 | 103906 |
| -8.40 | 120 | meas | $4-75^{\circ} \mathrm{C}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| -6.75 | 137.3 | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | A | 7.0034 |
| -2.80 | 1812.7 | A | $22.92341$ |  |  | B | $1458.21$ |
|  |  | B | $2708.38$ |  |  | C | 214.609 |
|  |  | C | 5.0 |  |  |  |  |

2. 

| Stull 1947 |  | Forziati et al. 1949 |  | Ambrose et al. 1967 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -6.9 | 133.3 | 59.335 | 6400 | 146.85 | 124200 | 28.24 | 1333 |
| 16.8 | 266.6 | 63.518 | 7692 | 166.85 | 202100 | 41.07 | 2666 |
| 28.3 | 1333 | 67.157 | 8991 | 186.85 | 313700 | 49.23 | 4000 |
| 41.1 | 2666 | 70.506 | 10330 | 206.85 | 467000 | 56.33 | 5333 |

TABLE 3.1.1.5.2 (Continued)

| Stull 1947 |  | Forziati et al. 1949 |  | Ambrose et al. 1967 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 55.3 | 5333 | 73.601 | 11720 | 226.85 | 671500 | 60.269 | 6666 |
| 64.4 | 7999 | 77.778 | 13842 | 246.85 | 937400 | 64.437 | 7999 |
| 76.8 | 13332 | 81.527 | 16633 | 266.85 | 1276300 | 71.277 | 10666 |
| 95.5 | 26664 | 87.387 | 19945 | 268.86 | 1700900 | 76.818 | 13332 |
| 116.7 | 53329 | 91.874 | 23474 | 306.85 | 2226600 | 87.454 | 19998 |
| 139.1 | 101325 | 97.887 | 28979 | 316.85 | 2872100 | 95.483 | 26664 |
|  |  | 103.412 | 34925 |  |  | 102.01 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -47.9 | 110.067 | 43360 | eq. 5 | P/bar | 107.55 | 39997 |
|  |  | 116.923 | 53700 | A | 21.9924 | 116.69 | 53329 |
|  |  | 124.226 | 66796 | B | 2957.79 | 124.15 | 66661 |
|  |  | 132.144 | 83749 | C | 5.66789 | 130.58 | 79993 |
|  |  | 137.731 | 97647 | D | 1776 | 136.06 | 93326 |
|  |  | 138.329 | 99235 |  |  | 137.1 | 95991 |
|  |  | 138.887 | 100726 |  |  | 138.112 | 98659 |
|  |  | 129.52 | 102464 |  |  | 138.1 | 101325 |
|  |  | 140.078 | 104000 |  |  | 25 | 1106.6 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{p} / \mathrm{mmHg}$ |
|  |  | A | 7.00849 |  |  | A | 7.00908 |
|  |  | B | 1461.925 |  |  | B | 1462.266 |
|  |  | C | 215.073 |  |  | C | 215.105 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 139.104 |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 139.103 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}}$ | $\left.\mathrm{mol}^{-1}\right)=$ |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 42.66 |
|  |  |  |  |  |  | at bp | 36.36 |



FIGURE 3.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for $m$-xylene.

TABLE 3.1.1.5.3
Reported Henry's law constants of $\boldsymbol{m}$-xylene at various temperatures and temperature dependence equations

| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | (2) | $\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| $\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(4)$ | $\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| $\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$ | (5) |  |


| Sanemasa et al. 1982 |  | Ashworth et al. 1988 |  | Robbins et al. 1993 |  | Dewulf et al. 1995 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| vapor-liquid equilibrium |  | EPICS-GC |  | static headspace-GC |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 15 | 405 | 10 | 416 | 25 | 739 | 2 | 209 |
| 25 | 731 | 15 | 503 | 30 | 900 | 6 | 204 |
| 35 | 1329 | 20 | 606 | 40 | 1489 | 10 | 264 |
| 45 | 1872 | 25 | 754 | 45 | 1591 | 18.2 | 472 |
|  |  | 30 | 899 | 50 | 1652 | 25 | 615 |
|  |  | eq. 4 a | $\mathrm{H} /(\mathrm{atm} \mathrm{m} 3 / \mathrm{mol})$ | eq. 4 | $\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ | eq 1 | $\mathrm{K}_{\text {AW }}$ |
|  |  | A | 6.28 | A | 17.83472 | A | 12.13 |
|  |  | B | 3337 | B | 3337.45 | B | 4026 |



FIGURE 3.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for $m$-xylene.

TABLE 3.1.1.5.4
Reported octanol-air partition coefficients of $m$-xylene at various temperatures

Gruber et al. 1997

|  | GC det'd activity coefficient |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\mathrm{OA}}$ |
| 20.29 | - |
| 30.3 | 3.69 |
| 40.4 | 3.51 |
| 50.28 | 3.30 |

### 3.1.1.6 p-Xylene



Common Name: $p$-Xylene
Synonym: 1,4-dimethylbenzene, $p$-xylol, 4-methyltoluene
Chemical Name: $p$-xylene
CAS Registry No: 106-42-3
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{10}, \mathrm{C}_{6} \mathrm{H}_{4}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 106.165
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): 13.25 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 138.37 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8611 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $123.3 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $42.376,35.98 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)
Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 17.113 (Tsonopoulos \& Prausnitz 1971; Riddick et al. 1986) 17.11 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 59.413 (Tsonopoulos \& Prausnitz 1971; Yalkowsky \& Valvani 1980) 59.77, 45.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
200 (shake flask-UV, Andrews \& Keefer 1949)
198* (shake flask-UV, measured range $0.4-85^{\circ} \mathrm{C}$, Bohon \& Claussen 1951)
185* (shake flask-GC, Polak \& Lu 1973)
156 (shake flask-GC, Sutton \& Calder 1975)
163 (shake flask-GC, Hermann 1972)
157 (shake flask-GC, Price 1976)
157 (shake flask-GC, Krzyzanowska \& Szeliga 1978)
191* ( $20^{\circ} \mathrm{C}$, shake flask-UV, Ben-Naim \& Wiff 1979)
163* (vapor saturation-UV spec., measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
214.5 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)

182 (HPLC-k' correlation, converted from reported $\gamma_{\mathrm{w}}$, Hafkenscheid \& Tomlinson 1983a)
214 (generator column-HPLC, Wasik et al. 1983)
215 (generator column-GC/ECD, Miller et al. 1985)
190 (shake flask-radiometric, Lo et al. 1986)
180* (IUPAC recommended value, temp range $0-90^{\circ} \mathrm{C}$, Shaw 1989b)
$169^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, equilibrium flow cell-GC, measured range $30-100^{\circ} \mathrm{C}$, Chen \& Wagner 1994c)
$\ln x=11.79-20.89 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-1}+4.892 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-2} ; \mathrm{T}_{\mathrm{r}}=\mathrm{T} / \mathrm{T}_{\mathrm{c}}$, the reduced temp, system temp T divided by critical temp $\mathrm{T}_{\mathrm{c}}$, temp range 303.15-373.15 K (equilibrium flow cell-GC, Chen \& Wagner 1994c)
$\ln x=-27.937+3230.3 /(\mathrm{T} / \mathrm{K})+7.595 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
154.7* $\quad\left(0.2^{\circ} \mathrm{C}\right.$, mercury manometer, Linder 1931)

787* $\quad\left(20^{\circ} \mathrm{C}, \mathrm{Hg}\right.$ manometer, Kassel 1936)
$\log (\mathrm{P} / \mathrm{mmHg})=-2930.0 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+23.1000$; temp range $0-80^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)
1437* $\quad\left(30^{\circ} \mathrm{C}, \mathrm{Hg}\right.$ manometer, measured range $10-50^{\circ} \mathrm{C}$, Rintelen et al. 1937)
$\log (\mathrm{P} / \mathrm{mmHg})=-2851.90 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+22.88436$; temp range $4-75^{\circ} \mathrm{C}$ (vapor pressure eq. from manometer measurement, Stuckey \& Saylor 1940)
1187* (Hg manometer, Pitzer \& Scott 1943)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=-3141.33 /(\mathrm{T} / \mathrm{K})+11.6092$; temp range $0-13.23^{\circ} \mathrm{C}$ (manometer, solid, two-constant vapor pressure eq. from exptl. data, Pitzer \& Scott 1943)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=-3080.31 /(\mathrm{T} / \mathrm{K})-6.7 \log (\mathrm{~T} / \mathrm{K})+27.8581$; temp range $13.23-60^{\circ} \mathrm{C}$ (manometer, liquid, threeconstant eq. from exptl. data, Pitzer \& Scott 1943)
$6354^{*} \quad\left(58.288^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $58.288-139.289^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98648-1491.548 /\left(207.171+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $58.3-139.8^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
$1333^{*} \quad\left(27.3^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6398^{*} \quad\left(58.419^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $58.419-139.329^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99184-1454.328 /\left(215.411+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $58.4-139.3^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
1175 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99052-1453.430 /\left(215.307+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $45-190^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$126500^{*} \quad\left(146.85^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $146.85-316.85^{\circ} \mathrm{C}$, Ambrose et al. 1967)
1170* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9052-1453,430 /\left(215.307+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $27.32-165.73^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9809.9 /(\mathrm{T} / \mathrm{K})]+8.124805$; temp range -8.1 to $138.3^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$880.3^{*} \quad\left(20.015^{\circ} \mathrm{C}\right.$, inclined-piston gauge, measured range -26.043 to 20.015 , Osborn \& Douslin 1974)
$\log (\mathrm{P} / \mathrm{atm})=(1-411.503 / \mathrm{T}) \times 10^{\wedge}\left(0.847730-6.39489 \times 10^{4} \cdot \mathrm{~T}+5.59094 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 290.0-618.2 K (Cox vapor pressure eq., Chao et al. 1983)

1170 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.11376-1452.215 /\left(215.518+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range $58.3-139.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.11513-1453.812 /\left(215.242+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $99.17-179.23^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Osborn \& Douslin 1974, Boublik et al. 1984)
1167 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.90052-1453.430 /\left(215.31+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $27-166^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
1200; 1160 (quoted lit.; calculated-Antoine eq., Riddick et al. 1986; quoted, Howard 1990)
$\log (\mathrm{P} / \mathrm{kPa})=6.11140-1451.39 /\left(215.148+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986)
1180 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=15.50091-6327.014 /(115.724+\mathrm{T} / \mathrm{K})$; temp range $247-286 \mathrm{~K}$ (solid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.14779-1475.767 /(-55.241+\mathrm{T} / \mathrm{K})$; temp range $286-453 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.14049-1472.773 /(-55.342+\mathrm{T} / \mathrm{K})$; temp range $411-463 \mathrm{~K}$ (liquid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.44333-1735.196 /(-19.846+\mathrm{T} / \mathrm{K})$; temp range $460-553 \mathrm{~K}$ (liquid, Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.84182-3543.356 /(208.522+\mathrm{T} / \mathrm{K})$; temp range $551-616 \mathrm{~K}$ (liquid, Antoine eq.-V, Stephenson \& Malanowski 1987)
1165* (McLeod gauge, measured range 20.0-50.07, Smith 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=60.0531-4.1059 \times 10^{3} /(\mathrm{T} / \mathrm{K})-19.441 \cdot \log (\mathrm{~T} / \mathrm{K})+8.2881 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-2.3647 \times 10^{-12} .(\mathrm{T} / \mathrm{K})^{2}$, temp range $286-616 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$762^{*} \quad$ (vapor-liquid equilibrium, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
754*; 752 (EPICS-GC/FID; batch air stripping-GC, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=6.931-3520 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
614 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
856, 1189, $1576 \quad\left(27,35.8,46^{\circ} \mathrm{C}\right.$, EPICS-GC, Hansen et al. 1993)
$\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-3072 /(\mathrm{T} / \mathrm{K})+10.0$; temp range $27-46^{\circ} \mathrm{C}($ EPICS measurements, Hansen et al. 1993)
696 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
739* (static headspace-GC, same as $m$-xylene, Robbins et al. 1993)
595 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
575* (EPICS-GC/FID, measured range $2-25^{\circ} \mathrm{C}$, Dewulf et al. 1995)
318, $763 \quad\left(6.0,25^{\circ} \mathrm{C}\right.$, EPICS-GC/FID, natural seawater with salinity of $35 \%$, Dewulf et al. 1995)
$\ln \mathrm{K}_{\mathrm{AW}}=-4479 /(\mathrm{T} / \mathrm{K})+0.01196 \cdot \mathrm{Z}+13.597$; with Z salinity $0-35.5 \%$ o, temp range $2-25^{\circ} \mathrm{C}(\mathrm{EPICS}-\mathrm{GC} / \mathrm{FID}$, Dewulf et al. 1995)
$641 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
678.6 (exponential saturator EXPSAT technique, Dohnal \& Hovorka 1999)
669.1 (modified EPICS method-GC, Ryu \& Park 1999)
$604 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=4.900-1615 /(\mathrm{T} / \mathrm{K})($ van’t Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ at $25^{\circ} \mathrm{C}$ :
3.15 (Leo et al. 1971; Hansch \& Leo 1985)
3.20 (Hansch \& Leo 1979)
3.10 (HPLC-k' correlation, Hanai et al. 1981)
3.28 (HPLC-k' correlation, Hammers et al. 1982)
3.18 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982b,c)
3.29 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983b)
3.18 (generator column-HPLC/UV, Wasik et al. 1983)
3.29 (HPLC-RV correlation, Garst 1984)
3.36, 3.48 (RP-HPLC-k' capacity factor correlations; Sherblom \& Eganhouse 1988)
3.15 (recommended, Sangster 1989, 1993)
3.35 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
3.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated

* are compiled at the end of this section:
3.68* $\quad\left(30.3^{\circ} \mathrm{C}\right.$, from GC-determined $\gamma^{\infty}$ in octanol, measured range $30.3-50.28^{\circ} \mathrm{C}$, Gruber et al. 1997)
3.79 (calculated-measured $\gamma^{\infty}$ in pure octanol of Gruber et al. 1997, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
1.37 (eels, Ogata \& Miyake 1978)
1.17 (goldfish, Ogata et al. 1984)
2.41 (S. capricornutum, Herman et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
2.52 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach \& Westall 1981)
2.42 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
2.24 (aquifer material with $\mathrm{f}_{\mathrm{OC}}$ of 0.006 and measured partition coeff. $\mathrm{K}_{\mathrm{P}}=1.04 \mathrm{~mL} / \mathrm{g}$., Abdul et al. 1990)
1.87, 2.22 (Webster soil, Webster soil HP, batch equilibrium, Pennell et al. 1992)
3.53, 2.63 (sorbent: Silica gel, kaolinite, batch equilibrium, Pennell et al. 1992)
2.72, 2.17 (Captina silt loam pH 4.97, McLaurin sandy loam pH 4.43, Walton et al. 1992)
2.43, 2.44 (RP-HPLC- $\mathrm{k}^{\prime}$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.37 (HPLC-screening method, Müller \& Kördel 1996)
2.49, 2.75, 2.65, 2.76, 2.79, 2.76, $2.78 \quad\left(2.3,3.8,6.2,8.0,13.5,18.6,25^{\circ} \mathrm{C}\right.$, natural sediment from River Leie, organic carbon $f_{\text {OC }}=4.12 \%$, EPICS-GC/FID, Dewulf et al. 1999)
2.27, 2.31, $2.21 \quad$ (soils: organic carbon $\mathrm{OC} \geq 0.1 \%, \mathrm{OC} \geq 0.5 \%, 0.1 \leq \mathrm{OC}<0.5 \%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $t_{1 / 2} \sim 3.1 \mathrm{~h}$ for evaporation from water of 1 m depth with wind speed of $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{sh}$ (Lyman et al. 1982);
$t_{1 / 2} \sim 27-135 \mathrm{~h}$ for evaporation from a typical river or pond (Howard 1990).
Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated. Additional data at other temperatures designated $*$ are compiled at the end of this section:
photooxidation $t_{1 / 2}=2.8 \times 10^{6}-1.4 \times 10^{8} \mathrm{~h}$, based on estimated rate data for alkoxy radical in aqueous solution (Hendry 1974)
$\mathrm{k}_{\mathrm{OH}}=(7.4 \pm 1.5) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(1.09 \pm 0.11) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(12.2 \pm 1.2) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(1.81 \pm 0.18) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}^{3} \mathrm{P}$ ) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=7.45 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(15.3 \pm 1.7) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured range $296-473 \mathrm{~K}$ (flash photolysisresonance fluorescence, Perry et al. 1977)
$\mathrm{k}_{\mathrm{OH}}=(8.8-10.5) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysisresonance fluorescence, Ravishanakara et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=12.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and residence time of 0.9 d , loss of $67 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=950 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at 300 K (Lyman et al. 1982)
$\mathrm{k}_{\text {OH }}=(5.9-12) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.47-1.0 \mathrm{~d}$ for xylenes (Mill 1982)
$\mathrm{k}=(140 \pm 30) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water using $1 \mathrm{mM} t$-BuOH as scavenger at pH 2.0 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{NO} 3}=1.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=14.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with half-life of $4.2-42 \mathrm{~h}$ (Atkinson 1985; Howard et al. 1991)
$\mathrm{k}_{\mathrm{OH}}=12.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $25^{\circ} \mathrm{C}$ (Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=13.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $22.8^{\circ} \mathrm{C}$, with a calculated atmospheric lifetime $\tau=0.84 \mathrm{~d}$ (Edney et al. 1986)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ obs. $)=15.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{NO} 3}=4.50 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=1.52 \times 10^{-11} \mathrm{~cm}^{3} \cdot \mathrm{molecule}^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}} *=1.43 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ over temp range at $296-335 \mathrm{~K}$ (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=14.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.92 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=17.40 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.51 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ exptl $)=14.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok \& Atkinson 1995)
Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982)
$\mathrm{t}_{1 / 2}=1150$ months, abiotic hydrolysis or dehydro-halogenation half-life (Olsen \& Davis 1990).
Biodegradation:
$100 \%$ biodegraded after 192 h at $13^{\circ} \mathrm{C}$ with an initial conen of $1.03 \times 10^{-6} \mathrm{~L} / \mathrm{L}$ (Jamison et al. 1976)
$\mathrm{t}_{1 / 2}$ (aq. aqueous) $=168-672 \mathrm{~h}$, based on aqueous screening test data (Bridie et al. 1979) and soil column study simulating an aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=672-2688 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)
$\mathrm{t}_{1 / 2}=0.03 \mathrm{~d}$ (Olsen \& Davis 1990).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976) residence time of 0.9 d , loss of $67 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
photodecomposition $t_{1 / 2}=3.1 \mathrm{~h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976)
$t_{1 / 2}=4.2-42 \mathrm{~h}$, based on photooxidation half-life (Howard et al. 1991);
calculated atmospheric lifetime $\tau=0.84 \mathrm{~d}$ due to reaction with OH radical (Edney et al. 1986);
summer daylight lifetime $\tau=10 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991).
Surface Water: $\mathrm{t}_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Ground water: $\mathrm{t}_{1 / 2}=336-8640 \mathrm{~h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991);
$\mathrm{t}_{1 / 2} \sim 0.3 \mathrm{yr}$ from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981); abiotic hydrolysis or dehydro-halogenation $\mathrm{t}_{1 / 2}=1150$ months (Olsen \& Davis 1990).
Soil: $\mathrm{t}_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);
disappearance $\mathrm{t}_{1 / 2}=2.2 \mathrm{~d}$ from test soils (Anderson et al. 1991).
Biota: $\mathrm{t}_{1 / 2}=2.6 \mathrm{~d}$, half-life to eliminate from eels in seawater (Ogata \& Miyake 1978).

TABLE 3.1.1.6.1
Reported aqueous solubilities of $\boldsymbol{p}$-xylene at various temperatures
1.

| Bohon \& Claussen 1951 |  | Polak \& Lu 1973 |  | Shaw 1989b (IUPAC) |  | Chen \& Wagner 1994c |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-GC |  | recommended values |  | equilibrium flow cell-GC |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\prime}{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0.4 | 156 | 0 | 164 | 0 | 160 | 30 | 169 |
| 10 | 188 | 25 | 185 | 10 | 200 | 30 | 188 |
| 10 | 197 |  |  | 20 | 180 | 50 | 102 |
| 21 | 195 |  |  | 25 | 180 | 60 | 230 |
| 25 | 198 |  |  | 30 | 190 | 70 | 289 |
| 25.6 | 199 | Ben-Nai | Wiff 1979 | 40 | 220 | 80 | 337 |
| 30.2 | 201 | shak | k-UV | 50 | 280 | 90 | 395 |
| 30.3 | 204 | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | 60 | 320 | 100 | 516 |
| 34.9 | 207 | 10 | 189 | 70 | 360 |  |  |
| 35.2 | 207 | 20 | 191 | 80 | 420 |  | $\left.\mathrm{ol}^{-1}\right)=3.48$ |
| 42.8 | 222 |  |  | 90 | 480 |  |  |
| 42.8 | 256 |  |  |  |  |  |  |
| 54.4 | 310 |  |  | $\Delta \mathrm{H}_{\text {sol }}$ | $\left.\mathrm{l}^{-1}\right)=6.90$ |  |  |
| 61.7 | 340 | Sanem | al. 1982 |  |  |  |  |
| 73.9 | 387 | vapor | tion-UV |  |  |  |  |
| 85 | 459 | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |  |  |  |  |
| $\Delta \mathrm{H}_{\text {sol }}\left(\mathrm{kJ} \mathrm{mol}{ }^{-1}\right)=$ |  | 15 | 157 |  |  |  |  |
| $25^{\circ} \mathrm{C}$ | 3.9 | 25 | 163 |  |  |  |  |
| $7^{\circ} \mathrm{C}$ | -0.422 | 35 | 176 |  |  |  |  |
| $12^{\circ} \mathrm{C}$ | -1.34 | 45 | 178 |  |  |  |  |
| $17^{\circ} \mathrm{C}$ | 0.515 | $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.20 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  |  |  |  |  |
| $22^{\circ} \mathrm{C}$ | 1.36 |  |  |  |  |  |  |
| $27^{\circ} \mathrm{C}$ | 2.29 |  |  |  |  |  |  |
| $32^{\circ} \mathrm{C}$ | 4.23 |  |  |  |  |  |  |
| $37^{\circ} \mathrm{C}$ | 7.36 |  |  |  |  |  |  |



FIGURE 3.1.1.6.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $p$-xylene.

TABLE 3.1.1.6.2
Reported vapor pressures of $\boldsymbol{p}$-xylene at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{align*}
& \log P=A-B /(T / K)  \tag{1a}\\
& \log P=A-B /\left(C+t /{ }^{\circ} C\right)  \tag{2}\\
& \log P=A-B /(C+T / K)  \tag{3}\\
& \log P=A-B /(T / K)-C \cdot \log (T / K)  \tag{4}\\
& \log P=A-B /(T / K)-C \cdot \log (T / K)+D(T / K)^{2} \tag{5}
\end{align*}
$$

$$
\text { (1) } \quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})
$$

$$
\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)
$$

1. 

| Kassel 1936 |  | Rintelen et al. 1937 |  | Pitzer \& Scott 1943 |  | Willingham et al. 1945 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer |  | mercury manometer |  | mercury manometer |  | ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 0 | 208 | 10 | 307 | 0 | 178 | 58.288 | 6354 |
| 10 | 415 | 30 | 1427 | 12.5 | 540 | 62.523 | 7657 |
| 20 | 787 | 50 | 4306 | 25 | 1187 | 66.216 | 8966 |
| 30 | 1427 |  |  | 37.7 | 2333 | 69.549 | 10306 |
| 40 | 2453 | bp 13 | $38.37^{\circ} \mathrm{C}$ | 50 | 4346 | 72.657 | 11696 |
| 50 | 4093 |  |  | 60 | 6846 | 76.832 | 13822 |
| 60 | 6573 |  |  |  |  | 81.636 | 16623 |
| 70 | 10226 |  |  |  |  | 86.488 | 18725 |
| 80 | 15452 |  |  | $0-13.23{ }^{\circ} \mathrm{C}$ solid |  | 90.990 | 23454 |
|  |  |  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | 97.013 | 28956 |
| eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | A | 11.6092 | 102.546 | 34901 |
| A | 23.100 |  |  | B | 3141.33 | 109.211 | 43326 |
| B | 2930.0 |  |  |  |  | 116.083 | 53656 |
| C | 5.0 |  |  | $13.23-60^{\circ} \mathrm{C}$ liquid |  | 123.049 | 66756 |
|  |  |  |  | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 131.355 | 83717 |
|  |  |  |  | A | 27.8581 | 136.956 | 97605 |
|  |  |  |  | B | 3080.31 | 137.558 | 99201 |

TABLE 3.1.1.6.2 (Continued)

2.

| Stull 1947 |  | Forziati et al. 1949 |  | Ambrose et al. 1967 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -8.10 | 133.3 | 58.419 | 6398 | 146.85 | 126500 | 27.32 | 1333 |
| 15.5 | 266.6 | 62.419 | 7690 | 166.85 | 205200 | 40.15 | 2666 |
| 27.3 | 1333 | 66.280 | 8990 | 186.85 | 317100 | 48.31 | 4000 |
| 40.1 | 2666 | 69.605 | 10330 | 206.85 | 470900 | 54.42 | 5333 |
| 54.4 | 5333 | 72.684 | 11720 | 226.85 | 675800 | 59.363 | 6666 |
| 63.5 | 7999 | 76.885 | 13842 | 246.85 | 941900 | 63.535 | 7999 |
| 75.9 | 13332 | 81.658 | 16633 | 266.85 | 1280800 | 70.383 | 10666 |
| 94.6 | 26664 | 86.506 | 19944 | 286.85 | 1705700 | 75.931 | 13332 |
| 115.9 | 53323 | 91.017 | 23474 | 306.85 | 2232400 | 86.583 | 19998 |
| 138.3 | 101325 | 97.032 | 28978 | 316.85 | 2880400 | 94.626 | 26664 |
|  |  | 102.573 | 34925 |  |  | 101.167 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 13.3 | 109.240 | 43360 | eq. 5 | P/bar | 106.719 | 39997 |
|  |  | 123.431 | 66796 | A | 21.14250 | 115.887 | 53329 |
|  |  | 131.371 | 83749 | B | 2892.27 | 123.366 | 66661 |
|  |  | 137.574 | 99235 | C | 5.40051 | 129.372 | 79993 |
|  |  | 138.132 | 100726 | D | 1759 | 135.304 | 93326 |
|  |  | 138.768 | 102462 |  |  | 136.341 | 95991 |
|  |  | 139.329 | 104000 |  |  | 137.347 | 98659 |
|  |  |  |  |  |  | 138.351 | 101325 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | 25.0 | 1173.2 |
|  |  | A | $6.99184$ |  |  |  |  |
|  |  | B | 1454.328 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | C | 215.411 |  |  | A | 6.99052 |
|  |  |  |  |  |  | B | 1453.430 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 138.351 |  |  | C | 215.307 |
|  |  |  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | $138.351$ |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 42.38 |
|  |  |  |  |  |  | at bp | 35.98 |
|  |  |  |  |  |  |  | (Continued) |

TABLE 3.1.1.6.2 (Continued)
3.

| Osborn \& Douslin 1974 |  |  |  | $\begin{gathered} \text { Smith } 1990 \\ \hline \text { McLeod gauge } \end{gathered}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| inclined-piston gauge |  | ebulliometry |  |  |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |
| -26.043 | 11.60 | 67.795 | 9590 | 20.0 | 865.3 |
| -21.164 | 19.60 | 70.881 | 10892 | 25.0 | 1165 |
| -16.277 | 33.20 | 73.978 | 12344 | 30.0 | 1541 |
| -10.403 | 60.79 | 77.086 | 13960 | 35.24 | 2075 |
| -4.995 | 103.86 | 80.206 | 15752 | 40.0 | 2645 |
| -0.006 | 170.5 | 83.339 | 17737 | 44.27 | 3306 |
| 4.912 | 272.4 | 86.483 | 19933 | 50.07 | 4374 |
| 9.838 | 429.2 | 92.804 | 25023 |  |  |
| 12.483 | 544.4 |  |  |  |  |
| 13.285 | 581.7 |  |  | eq. 2 a | P/mmHg |
| 15.004 | 648.9 |  |  | A | 16.19136 |
| 17.474 | 755.4 |  |  | B | 3371.18 |
| 20.015 | 880.3 |  |  | C | 215.367 |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{k}$ | $\left.\mathrm{l}^{-1}\right)=42.98$ |
|  |  |  |  |  |  |
|  |  |  |  | $\Delta \mathrm{S}_{\mathrm{v}} /(\mathrm{J} \mathrm{n}$ | $\left.\mathrm{K}^{-1}\right)=107.0$ |



FIGURE 3.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for $p$-xylene.

## TABLE 3.1.1.6.3

Reported Henry's law constants of $\boldsymbol{p}$-xylene at various temperatures and temperature dependence equations

$$
\begin{align*}
& \ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1a}\\
& \ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{2a}\\
& \ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{3}\\
& \ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{~m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{4a}\\
& \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{~T} / \mathrm{K})^{2} \tag{5}
\end{align*}
$$

$$
\text { (1) } \quad \log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})
$$

(2) $\quad \log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(4) $\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

| Sanemasa et al. 1982 |  | Ashworth et al. 1988 |  | Robbins et al. 1993 |  | Hansen et al. 1993 |  | Dewulf et al. 1995 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| vapor-liquid equil |  | EPICS-GC |  | static headspace-GC |  | EPICS-GC |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/Pa m ${ }^{3} / \mathrm{mol}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/Pa m ${ }^{3} / \mathrm{mol}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/Pa m ${ }^{3} / \mathrm{mol}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/Pa m ${ }^{3} / \mathrm{mol}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/Pa m ${ }^{3} / \mathrm{mol}$ |
| 15 | 430 | 10 | 426 | 25 | 739 | 27 | 856 | 2 | 176 |
| 25 | 762 | 15 | 489 | 30 | 900 | 35.8 | 1189 | 6 | 158 |
| 35 | 1265 | 20 | 654 | 40 | 1489 | 46 | 1576 | 10 | 252 |
| 45 | 2052 | 25 | 754 | 45 | 1591 |  |  | 18.2 | 468 |
|  |  | 30 | 958 | 50 | 1652 |  |  | 25 | 575 |
|  |  |  | eq. 4 a |  | eq. 4 |  | eq. 4 | eq 1 | $\mathrm{K}_{\text {AW }}$ |
|  |  |  | tm m $3 / \mathrm{mol}$ ) |  | a $\mathrm{m}^{3} / \mathrm{mol}$ ) |  | $\mathrm{Pa} \mathrm{m} / \mathrm{mol})$ | A | 13.597 |
|  |  | A | 6.931 | A | 17.83472 | A | 10.1 | B | 4479 |
|  |  | B | 3520 | B | 3337.45 | B | 3072 |  |  |



FIGURE 3.1.1.6.3 Logarithm of Henry's law constant versus reciprocal temperature for $p$-xylene.

## TABLE 3.1.1.6.4

Reported octanol-air partition coefficients of $p$ xylene at various temperatures

Gruber et al. 1997

|  | GC det'd activity coefficient |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\mathrm{OA}}$ |
| 20.29 | - |
| 30.3 | 3.68 |
| 40.4 | 3.48 |
| 50.28 | 3.29 |

### 3.1.1.7 1,2,3-Trimethylbenzene



Common Name: 1,2,3-Trimethylbenzene
Synonym: hemimellitene
Chemical Name: 1,2,3-trimethylbenzene
CAS Registry No: 526-73-8
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{3}\left(\mathrm{CH}_{3}\right)_{3}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -25.4 (Weast 1982-83; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
176.1 (Weast 1982-83; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8944 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $134.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : $0.66,1.33,8.18 ; 10.17 \quad\left(-54.45,-42.85,-25.35^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 41.81, 46.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
75.2 (shake flask-GC, Sutton \& Calder 1975)
62.7* (vapor saturation-UV spec., measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
65.5 (generator column-HPLC/UV, Tewari et al. 1982c)

69* (IUPAC recommended value, temp range $15-45^{\circ} \mathrm{C}$, Shaw 1989b)
$\ln x=-39.5173+5289.13 /(\mathrm{T} / \mathrm{K})+1.149 \times 10^{-4} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section):
133.3* $\quad\left(16.8^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6417^{*} \quad\left(90.332^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $90.332-177.126^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04082-1593.958 /\left(207.078+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $90.3-177.1^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
206 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04082-1593.958 /\left(207.078 \mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-230^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
198* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04082-1593.958 /\left(207.078+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $56.79-205.36^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10781.9 /(\mathrm{T} / \mathrm{K})]+8.154069$; temp range $16.8-176^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 217 (calculated-bp, Mackay et al. 1982; Eastcott et al. 1988)
$\log (\mathrm{P} / \mathrm{atm})=(1-449.175 / \mathrm{T}) \times 10^{\wedge}\left(0.869047-6.33423 \times 10^{4} \cdot \mathrm{~T}+5.14963 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 290.0-660.0 K (Cox vapor pressure eq., Chao et al. 1983)

157 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.16365-1592.422 /\left(206.905+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $90.33-177.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
198.4 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04082-1593.958 /\left(207.08+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $57-205^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
199 (extrapolated, Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16477-1593.776 /(-66.032+\mathrm{T} / \mathrm{K})$; temp range $363-456 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=2.7492-2.6428 \times 10^{3} /(\mathrm{T} / \mathrm{K})+3.6120 \cdot \log (\mathrm{~T} / \mathrm{K})-1.0213 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+5.0553 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 248-665 K (vapor pressure eq., Yaws 1994)
$\log (\mathrm{P} / \mathrm{kPa})=6.17303-1593.958 /[(\mathrm{T} / \mathrm{K})-66.072]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
441* (vapor-liquid equilibrium-GC, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
364 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
3.66 (Hansch \& Leo 1979)
3.66 (HPLC-k' correlation, Hammers et al. 1982)
3.55 (generator column-HPLC/UV, Tewari et al. 1982b, 1982c)
3.70, 3.86 (RP-HPLC-k' correlation, Sherblom \& Eganhouse 1988)
3.63 (recommended, Sangster 1989, 1993)
3.55, 3.59, 3.66 (quoted lit. values, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
2.80 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach \& Westall 1981)

Environmental Fate Rate Constants, $k$, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k ; for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=(14 \pm 3) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(6.9 \pm 0.7) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(26.4 \pm 2.6) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=11.5 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=14.9 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(33.3 \pm 4.5) \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured range $296-473 \mathrm{~K}$ (flash photolysisresonance fluorescence Perry et al. 1977)
$\mathrm{k}_{\mathrm{OH}}=(15-30) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.2-0.4 \mathrm{~d}$ for trimethylbenzenes (Mill 1982)
$\mathrm{k}=(400 \pm 100) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water at pH 1.7 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{NO} 3}=5.6 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=3.16 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=2.96 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=1.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.3.33 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{NO} 3}=1.85 \times 10^{-15} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=3.16 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}=3.27 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=1.78 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992
$\mathrm{k}_{\mathrm{OH}}($ calc $)=3.99 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biotransformation:
Biodegradation:
Bioconcentration:
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);
estimated lifetime $\tau=1.5 \mathrm{~h}$ under photochemical smog conditions in S.E. England (Brice \& Derwent 1978) and (Perry et al. 1977);
summer daylight lifetime $\tau=4.2 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991)

## TABLE 3.1.1.7.1

Reported aqueous solubilities and Henry's law constants of 1,2,3-trimethylbenzene at various temperatures

| Aqueous solubility |  |  |  | Henry's law constant <br> Sanemasa et al. 1982 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Sanemasa et al. 1982 |  | Shaw 1989b (IUPAC) |  |  |  |
| vapor saturation-UV |  | recommended values |  | vapor-liquid equilibrium |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 15 | 75.2 | 15 | 60 | 15 | 241.2 |
| 25 | 65.5 | 25 | 69 | 25 | 441 |
| 35 | 72.2 | 35 | 72 | 35 | 706 |
| 45 | 85.2 | 45 | 85 | 45 | 1058 |



FIGURE 3.1.1.7.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,3-trimethylbenzene.

TABLE 3.1.1.7.2
Reported vapor pressures of 1,2,3-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |


| Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 16.8 | 133.3 | 90.332 | 6417 | 56.79 | 1333 |
| 42.9 | 666.6 | 94.826 | 7697 | 70.62 | 2666 |
| 55.9 | 1333 | 98.77 | 8993 | 79.41 | 4000 |
| 69.9 | 2666 | 102.336 | 10328 | 86 | 5333 |
| 85.4 | 5333 | 105.663 | 11720 | 91.313 | 6666 |
| 95.3 | 7999 | 110.157 | 13840 | 95.802 | 7999 |
| 1088 | 13332 | 115.287 | 16640 | 103.168 | 10666 |
| 129 | 26664 | 120.504 | 19944 | 109.132 | 13332 |
| 152 | 53329 | 125.333 | 23474 | 120.578 | 19998 |
| 176.1 | 101325 | 131.8 | 28978 | 129.215 | 26664 |
|  |  | 137.737 | 34918 | 136.214 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -25.5 | 144.882 | 43351 | 142.191 | 39997 |
|  |  | 152.26 | 53692 | 152.022 | 53329 |
|  |  | 160.106 | 66792 | 160.037 | 66661 |
|  |  | 168.614 | 83750 | 166.856 | 79993 |
|  |  | 174.606 | 97644 | 172.823 | 93326 |
|  |  | 175.252 | 99237 | 173.934 | 95992 |
|  |  | 175.852 | 100732 | 175.02 | 98659 |
|  |  | 176.527 | 102453 | 176.084 | 101325 |
|  |  | 177.126 | 103985 |  |  |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  | A | 7.04082 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | B | 1593.958 |
|  |  | A | 7.04082 | C | 207.078 |
|  |  | B | 1593.958 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 176.084 |
|  |  | C | 207.078 | $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ} \mathrm{mo} \\ & \text { at } 25^{\circ} \mathrm{C} \end{aligned}$ | $\text { ) }=$ |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 176.084 | at bp | 40.04 |



FIGURE 3.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3-trimethylbenzene.

### 3.1.1.8 1,2,4-Trimethylbenzene



Common Name: 1,2,4-Trimethylbenzene
Synonym: pseudocumene
Chemical Name: 1,2,4-trimethylbenzene
CAS Registry No: 95-63-6
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{3}\left(\mathrm{CH}_{3}\right)_{3}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -43.77 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 169.38 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8758 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $137.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 13.19 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 57.53, 46.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):

```
57 (shake flask-GC, McAuliffe 1966)
59.0 (shake flask-GC, Sutton & Calder 1975)
51.9 (shake flask-GC, Price 1976)
51.9 (shake flask-GC, Krzyzanowska & Szeliga 1978)
56.5* (vapor saturation-UV spec., measured range 15-45 ' C, Sanemasa et al. 1982)
56* (IUPAC recommended, temp range 15-45*'C, Shaw 1989b)
ln}x=-8.760-868.70/(T/K); temp range 5-50 ' C (regression eq. of literature data, Shiu & Ma 2000)
```

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
133.3* $\quad\left(13.6^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6417^{*} \quad\left(84.804^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $84.804-170.377^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04393-1573.267 /\left(208.564+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $84.8-170.4^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
280 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04383-1573.267 /\left(208.564+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70-220^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
2666* $\quad\left(65.405^{\circ} \mathrm{C}\right.$, compiled data, temp range $65.405-198.215^{\circ} \mathrm{C}$, Bond \& Thodos 1960 )
$\log (\mathrm{P} / \mathrm{mmHg})=23.2393-3301.19 /(\mathrm{T} / \mathrm{K})-6.21412 \cdot \log (\mathrm{~T} / \mathrm{K})+3.15835\left[\mathrm{P}(\mathrm{mmHg}) /(\mathrm{T} / \mathrm{K})^{2}\right]$, temp range $65.4-198^{\circ} \mathrm{C}$ (Bond \& Thodos 1960)
271* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971; quoted, Mackay \& Shiu 1981; Eastcott et al. 1988)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04383-1573.267 /\left(208.564+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $51.75-198.2^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10710.2 /(\mathrm{T} / \mathrm{K})]+8.209013$; temp range $13.6-169.2^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) $\log (\mathrm{P} / \mathrm{atm})=(1-442.537 / \mathrm{T}) \times 10^{\wedge}\left(0.846724-5.41424 \times 10^{4} \cdot \mathrm{~T}+4.22211 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 253.0-645.0 K (Cox vapor pressure eq., Chao et al. 1983)

270 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.16282-1569.06 /\left(208.089+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $84.8-170.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04383-1573.83 /\left(208.56+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $52-198^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16695-1572.687 /(-64.593+\mathrm{T} / \mathrm{K})$; temp range $357-450 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=2.1667-2.6318 \times 10^{3} /(\mathrm{T} / \mathrm{K})+4.0350 \cdot \log (\mathrm{~T} / \mathrm{K})-1.1776 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+6.0956 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $229-649 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$\log (\mathrm{P} / \mathrm{kPa})=6.16866-1573.267 /[(\mathrm{T} / \mathrm{K})-64.586]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
619* (vapor-liquid equilibrium, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
$475 \quad\left(20^{\circ} \mathrm{C}\right.$, EPICS-GC, Yurteri et al. 1987)
571 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
$704,1135,1591 \quad\left(27,35,45^{\circ} \mathrm{C}\right.$, EPICS-GC, Hansen et al. 1993)
$\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-4298 /(\mathrm{T} / \mathrm{K})+14.0$; temp range $27-45^{\circ} \mathrm{C}$ (EPICS-GC, Hansen et al. 1993)
$529 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts, 1996, 2001) $\log \mathrm{K}_{\mathrm{AW}}=5.125-1697 /(\mathrm{T} / \mathrm{K})($ van't Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.65 (calculated $-\pi$ substituent constant, Hansch et al. 1968)
3.63 (shake flask-HPLC/UV both phases, Wasik et al. 1981)
3.78 (HPLC-k' correlation, Hammers et al. 1982)
3.82, 4.00 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
3.63 (recommended value, Sangster 1989)
3.78 (normal phase HPLC- $\mathrm{k}^{\prime}$ correlation, Govers \& Evers 1992)
3.70 (recommended, Sangster 1993)
3.83, 3.78 (quoted lit., Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.28 (computed- $\mathrm{K}_{\mathrm{OW}}$, Kollig 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Photolysis: rate constant $\mathrm{k}=2.686 \times 10^{-2} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with HO- in the gas (Dilling et al. 1988).
no photolyzable functional groups (Howard et al. 1991).
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{OH}}=(2.0 \pm 0.3) \times 10^{10} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.58 \mathrm{~h} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(6.0 \pm 0.6) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(33.5 \pm 3.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{NO} 3}=10.0 \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=20 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}^{*}=(40.0 \pm 4.5) \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured range $296-473 \mathrm{~K}$ (flash photolysisresonance fluorescence Perry et al. 1977)
photooxidation $t_{1 / 2}=1056-43000 \mathrm{~h}$ in water, based on measured rate data with hydroxy radical in aqueous solution (Güesten et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=33.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and residence time of 0.3 d , loss of $96.4 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=(1.5-30) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.2-0.4 \mathrm{~d}$ for trimethylbenzenes (Mill 1982)
$\mathrm{k}_{\mathrm{NO} 3}=5.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=38.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1.6-16 \mathrm{~h}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=31.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $25^{\circ} \mathrm{C}$ (Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=18 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ obs. $)=40 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{NO} 3}=1.80 \times 10^{-15} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{OH}}=3.84 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}} \approx 32.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=1.78 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=39.72 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).
Biodegradation: aqueous aerobic biodegradation $\mathrm{t}_{1 / 2}=168-672 \mathrm{~h}$, based on aqueous screening studies (Marion $\&$ Malaney 1964; Kitano 1978; Van der Linden 1978; Tester \& Harker 1981; Trzilova \& Horska 1988; Howard et al. 1991);
anaerobic aqueous biodegradation $t_{1 / 2}=672-2688 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.58 \mathrm{~h}$ estimated from the rate of disappearance for the reaction with OH radical (Doyle et al. 1975)
$\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976);
residence time of 0.3 d , loss of $96.4 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{t}_{1 / 2}=1.6-16 \mathrm{~h}$, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);
summer daylight lifetime $\tau=4.3 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991);
calculated lifetimes of $4.3 \mathrm{~h}, 26 \mathrm{~d}$ and $>4.5 \mathrm{yr}$ for reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$, respectively (Atkinson 2000).
Surface Water: $\mathrm{t}_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Kitano 1978; Van der Linden 1978; Tester \& Harker 1981; Trzilova \& Horska 1988; Marion \& Melaney 1964; Howard et al. 1991);
photooxidation $\mathrm{t}_{1 / 2}=1056-43000 \mathrm{~h}$, based on measured rate data with OH radical in aqueous solution (Güesten et al. 1981; Howard et al. 1991).
Ground water: $\mathrm{t}_{1 / 2}=336-1344 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Soil: $t_{1 / 2}=168-672 \mathrm{~h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Biota:

TABLE 3.1.1.8.1
Reported aqueous solubilities and Henry's law constants of $\mathbf{1 , 2 , 4 t r i m e t h y l b e n z e n e ~ a t ~ v a r i o u s ~ t e m p e r a t u r e s ~}$

| Aqueous solubility |  |  |  | Henry's law constant |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Sanemasa et al. 1982 |  | Shaw 1989b (IUPAC) |  | Sanemasa et al. 1982 |  | Hansen et al. 1993 |  |
| vapor saturation-UV |  | recommended values |  | vapor-liquid equilibrium |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 15 | 52.3 | 15 | 52 | 15 | 377 | 27 | 704 |
| 25 | 56.5 | 25 | 56 | 25 | 619 | 35 | 1135 |
| 35 | 62.1 | 35 | 62 | 35 | 1042 | 45 | 1591 |
| 45 | 69.3 | 45 | 69 | 45 | 1663 |  |  |
|  |  |  |  |  |  |  | $\begin{aligned} & \left.\left.\mathrm{kPa} \mathrm{~m}^{3} / \mathrm{mol}\right)\right]= \\ & \mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \end{aligned}$ |
|  |  |  |  |  |  | A | 14.0 |
|  |  |  |  |  |  | B | 4298 |



FIGURE 3.1.1.8.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,4-trimethylbenzene.

TABLE 3.1.1.8.2
Reported vapor pressures of 1,2,4-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \cdot \mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}$ | (5) |  |

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \cdot \mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}$
Stull 1947
Forziati et al. 1949

| summary of literature data |  |  | ebulliometry |  |  |
| :--- | :---: | :--- | :--- | :--- | :--- |
| $\mathbf{n} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ |  | $\mathbf{P} / \mathbf{P a}$ |
| 13.6 | 133.3 |  | 84.804 | 6417 |  |
| 38.4 | 666.6 |  | 89.259 | 7697 |  |
| 50.7 | 1333 |  | 93.155 | 8991 |  |
| 64.5 | 2666 |  | 96.65 | 10328 |  |

Bond \& Thodos 196
Zwolinski \& Wilhoit 1971
summary of literature data

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :---: | :---: | ---: | :---: |
| 65.405 | 2666 | 51.75 | 1333 |
| 97.49 | 10666 | 65.39 | 2666 |
| 153.55 | 66661 | 74.05 | 4000 |
| 180.505 | 133322 | 80.54 | 5333 |

TABLE 3.1.1.8.2 (Continued)

| Stull 1947 |  | Forziati et al. 1949 |  | Bond \& Thodos 1960 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | summary of literature data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 79.8 | 5333 | 99.94 | 11720 | 198.215 | 199984 | 85.787 | 6666 |
| 89.5 | 7999 | 104.369 | 13840 |  |  | 90.214 | 7999 |
| 102.8 | 13332 | 109.418 | 16640 | bp/ ${ }^{\circ} \mathrm{C}$ | 169.366 | 97.475 | 10666 |
| 122.7 | 26664 | 114.572 | 19944 |  |  | 103.355 | 13332 |
| 145.4 | 53329 | 119.328 | 23474 | eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | 114.639 | 19998 |
| 169.2 | 101325 | 125.694 | 28978 | A | 23.2393 | 123.153 | 26664 |
|  |  | 131.556 | 34918 | B | 3301.19 | 130.072 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -44.1 | 138.599 | 43351 | C | 6.21412 | 135.944 | 39997 |
|  |  | 145.867 | 53692 | D | 3.15835 | 145.634 | 53329 |
|  |  | 153.604 | 66792 |  |  | 153.534 | 66661 |
|  |  | 161.991 | 83750 |  |  | 160.256 | 79993 |
|  |  | 167.896 | 97644 |  |  | 166.137 | 93326 |
|  |  | 168.534 | 99237 |  |  | 167.231 | 95992 |
|  |  | 169.121 | 100732 |  |  | 168.302 | 98659 |
|  |  | 169.788 | 102453 |  |  | 169.351 | 101325 |
|  |  | 170.377 | 103985 |  |  |  |  |
|  |  |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | A | 7.04383 |
|  |  | A | 7.04383 |  |  | B | 1573.267 |
|  |  | B | 1573.267 |  |  | C | 208.564 |
|  |  | C | 208.564 |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | $169.351$ |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}}$ | $\left.\mathrm{JJ} \mathrm{mol}^{-1}\right)=$ |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 169.351 |  |  | at $25^{\circ} \mathrm{C}$ | 47.94 |
|  |  |  |  |  |  | at bp | 39.25 |



FIGURE 3.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4-trimethylbenzene.

### 3.1.1.9 1,3,5-Trimethylbenzene



Common Name: 1,3,5-Trimethylbenzene
Synonym: mesitylene
Chemical Name: 1,3,5-trimethylbenzene
CAS Registry No: 108-67-8
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{3}\left(\mathrm{CH}_{3}\right)_{3}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-44.7 (Weast 1982-83; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
164.74 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.880 \quad$ (Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $136.6 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
47.48, $39.04 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986) 51.85 (calculated-bp, Govers \& Evers 1992)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$9.514 \quad$ (Riddick et al. 1986)
9.51 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 41.66, 46.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
173 (residue-volume method, Booth \& Everson 1948)
97 (shake flask-UV, Andrews \& Keffer 1950)
39.4 (shake flask-UV, Vesala 1974)
48.2 (shake flask-GC, Sutton \& Calder 1975)
49.5* (vapor saturation-UV, temp range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1981)

50* (vapor saturation-UV, temp range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
49.5 (HPLC-k' correlation, converted from reported $\gamma_{\mathrm{W}}$, Hafkenscheid \& Tomlinson 1983)
48.9* (recommended, temp range $15-45^{\circ} \mathrm{C}$, Shaw 1989b)

64* $\quad\left(30^{\circ} \mathrm{C}\right.$, equilibrium flow cell-GC, measured range $30-100^{\circ} \mathrm{C}$, Chen \& Wagner 1994 c$)$
$\ln x=26.26-35.26 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-1}+7.905 \cdot\left(\mathrm{~T}_{\mathrm{r}} / \mathrm{K}\right)^{-2} ; \mathrm{T}_{\mathrm{r}}=\mathrm{T} / \mathrm{T}_{\mathrm{c}}$, the reduced temp, system temp T divided by critical temp $\mathrm{T}_{\mathrm{c}}$, temp range $303.15-373.15 \mathrm{~K}$ (equilibrium flow cell-GC, Chen \& Wagner 1994c)
$\ln x=-9.533-678.83 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$121.3^{*} \quad\left(10.6^{\circ} \mathrm{C}\right.$, mercury manometer, Linder 1931)
$248^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, mercury manometer, Kassel 1936)
$\log (\mathrm{P} / \mathrm{mmHg})=-3104.5 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+23.1929$; temp range $0-80^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Kassel 1936)
$507^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, mercury manometer, measured range $10-50^{\circ} \mathrm{C}$, Rintelen et al. 1937)
$\log (\mathrm{P} / \mathrm{mmHg})=-3122.45 /(\mathrm{T} / \mathrm{K})-5 \cdot \log (\mathrm{~T} / \mathrm{K})+22.23680$; temp range $4-75^{\circ} \mathrm{C}$ (manometer, vapor pressure eq. from exptl. data, Stuckey \& Saylor 1940)
$133.3^{*} \quad\left(9.6^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6415^{*} \quad\left(81.488^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $81.488-165.725^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=7.07437-1569.622 /\left(209.578+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $81.5-165.7^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
331 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.07436-1569.622 /\left(209.578+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70-210^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
328* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971; quoted, Mackay \& Shiu 1981; Eastcott et al. 1988)
$\log (\mathrm{P} / \mathrm{mmHg})=7.07435-1569.622 /\left(209.578+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $48.82-193.07^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10516.8 /(\mathrm{T} / \mathrm{K})]+8.161663$; temp range $9.6-164.7^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 366 (calculated-bp, Mackay et al. 1982)
$\log (\mathrm{P} / \mathrm{atm})=(1-437.769 / \mathrm{T}) \times 10^{\wedge}\left(0.872945-6.55508 \times 10^{4} \cdot \mathrm{~T}+5.47586 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 253.0-635.0 K (Cox vapor pressure eq., Chao et al. 1983)

323 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.20212-1571.575 /\left(209.79+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $81.488-165.7^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
322 (extrapolated-Antoine eq., Dean 1985)
330 (selected lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.21017-1577.80 /\left(210.526+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) $\log (\mathrm{P} / \mathrm{mmHg})=7.07436-1569.622 /\left(209.58+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $49-193^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
330 (interpolated-Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.19762-1569.749 /(-63.565+\mathrm{T} / \mathrm{K})$; temp range $354-445 \mathrm{~K}$ (liquid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.62312-1810.653 /(-43.307+\mathrm{T} / \mathrm{K})$; temp range $249-356 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson \& Malanowski 1987)
360 (computed-expert system SPARC, Kollig 1995)
$\log (\mathrm{P} / \mathrm{kPa})=6.18965-1569.622 /[(\mathrm{T} / \mathrm{K}) \pm 63.572]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
929* (vapor-liquid equilibrium, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1981)
887* (vapor-liquid equilibrium, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
682; 849 (EPICS; batch stripping, Ashworth et al. 1988)
682* (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988)
$\ln [\mathrm{H} /(\mathrm{atm} \mathrm{m} 3 / \mathrm{mol})]=7.241-3628 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
803 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
704 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
$597 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=4.329-1448 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
3.42 (Leo et al. 1971; Hansch \& Leo 1979)
3.78 (HPLC-k' correlation, Hammers et al. 1982)
3.82 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
3.42 (HPLC-RV correlation, Garst 1984)
3.89 (normal phase HPLC- $\mathrm{k}^{\prime}$ correlation, Govers \& Evers 1992)
3.42 (recommended value, Sangster 1993)
3.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
2.82 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach \& Westall 1981)
2.77 (soil, calculated-MCI $\chi$, Sabljic 1987a)
2.75 (soil, calculated-MCI $\chi$, Sabljic 1987b)
2.85 (soil, calculated-MCI $\chi$, Bahnick \& Doucette 1988)
2.82 (soil, calculated-QSAR- $\chi$, Sabljic et al. 1995)
3.37 (computed-K ${ }_{\text {ow }}$, Kollig 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: rate constant $\mathrm{k}=1.606 \times 10^{-2} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with HO in the gas (Dilling et al. 1988).
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
$\mathrm{k}_{\mathrm{O} 3}<60 \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for vapor phase reaction with ozone at $30^{\circ} \mathrm{C}$ (Bufalini \& Altshuller 1965)
$\mathrm{k}_{\mathrm{OH}}=(31 \pm 4) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(16.8 \pm 2.0) \times 10^{8} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\left.\mathrm{O}^{( }{ }^{3} \mathrm{P}\right)$ atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(47.2 \pm 4.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{O}(3 \mathrm{P})}=(27.9 \pm 3.3) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the reaction of $\mathrm{O}\left({ }^{3} \mathrm{P}\right)$ atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)
$\mathrm{k}_{\mathrm{OH}}=29.7 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=(62.4 \pm 7.5) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp., measured range 296-473 K (flash photolysisresonance fluorescence, Perry et al. 1977)
photooxidation in water, $\mathrm{t}_{1 / 2}=3208-1.28 \times 10^{5} \mathrm{~h}$, based on measured rate constant for reaction with hydroxyl radical in water (Mill et al. 1980)
$\mathrm{k}_{\mathrm{OH}}=49.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and residence time of 0.2 d , loss of $99.3 \%$ in one day or 12 sunlit hour at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{03}=4200 \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone at 300 K (Lyman et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=(15-30) \times 10^{9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.2-0.4 \mathrm{~d}$ for trimethylbenzenes (Mill 1982)
$\mathrm{k}=(700 \pm 200) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water at pH 1.7 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{NO} 3}=2.4 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=60.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=38.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{NO} 3}=7.91 \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{OH}}=6.05 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1985; Atkinson et al. 1988; quoted, Sabljic \& Güsten 1990; Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=38 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ obs. $)=62.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}} *=57.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=3.72 \times 10^{-11} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 298 K (estimated by SARs, Müller \& Klein 1992)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=54.16 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biodegradation: unacclimated aerobic aqueous biodegradation $t_{1 / 2}=48-192 \mathrm{~h}$, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler \& Wuhrmann 1978; Howard et al. 1991); $\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=192-768 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Bioconcentration:
Half-Lives in the Environment:
Air: 0.24-2.4 h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);
estimated lifetime under photochemical smog conditions in S.E. England is 0.7 h (Brice \& Derwent 1978; Perry et al. 1977 and Darnall et al. 1976);
residence time of 0.2 d , loss of $99.3 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{t}_{1 / 2}=9.72-97.2 \mathrm{~h}$, based on estimated photooxidation half-life in air (Atkinson 1987).
Surface Water: $t_{1 / 2}=48-192 \mathrm{~h}$, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler \& Wuhrmann 1978; Howard et al. 1991);
$t_{1 / 2}=1 \mathrm{~d}$ in surface waters in case a first order reduction process may be assumed (estimated, Zoeteman et al. 1980).
Ground water: $t_{1 / 2}=96-384 \mathrm{~h}$, based on a soil column study in which aerobic ground water was continuously percolated through quartz sand (Kappeler \& Wuhrmann 1978; Howard et al. 1991).
Soil: $t_{1 / 2}=48-192 \mathrm{~h}$, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler \& Wuhrmann 1978; Howard et al. 1991).
Biota:

TABLE 3.1.1.9.1
Reported aqueous solubilities of 1,3,5-trimethylbenzene at various temperatures

| Sanemasa et al. 1981 |  | Sanemasa et al. 1982 |  | Shaw 1989b (IUPAC) |  | Chen \& Wagner 1994c |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| vapor saturation-UV |  | vapor saturation-UV |  | recommended values |  | shake flask-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 15 | 45.6 | 15 | 46 | 15 | 46 | 30 | 64 |
| 25 | 49.5 | 25 | 50 | 25 | 48.9 | 40 | 67.8 |
| 35 | 54.2 | 35 | 54.9 | 35 | 54 | 50 | 74.12 |
| 45 | 56.5 | 45 | 58.9 | 45 | 57 | 60 | 90.82 |
|  |  |  |  |  |  | 70 | 111 |
|  |  |  |  |  |  | 80 | 140 |
|  |  |  |  |  |  | 90 | 164 |
|  |  |  |  |  |  | 100 | 194 |
|  |  |  |  |  |  | $\Delta \mathrm{H}$ | $\left.{ }^{-1}\right)=4.49$ |
|  |  |  |  |  |  |  |  |



FIGURE 3.1.1.9.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1,3,5-trimethylbenzene.

TABLE 3.1.1.9.2
Reported vapor pressures of $1,3,5$-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
1.

| Linder 1931 |  | Kassel 1936 |  | Rintelen et al. 1937 |  | Stull 1947 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Hg manometer |  | mercury manometer |  | mercury manometer |  | summary of literature data |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| -1.7 | 45.3 | 0 | 58.7 | 10 | 80 | 9.6 | 133.3 |
| 0 | 50 | 10 | 124 | 30 | 507 | 34.7 | 266.6 |
| 2.3 | 66.7 | 20 | 248 | 50 | 1523 | 47.4 | 1333 |
| 3.2 | 70.7 | 30 | 521 | Stuckey | aylor 1940 | 61 | 2666 |
| -2.75 | 38.66 | 40 | 844 | mercu | anometer | 76.1 | 5333 |
| -1.20 | 44 | 50 | 1467 | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | 85.8 | 7999 |
| 1.5 | 57.3 | 60 | 2440 | mea | $4-75^{\circ} \mathrm{C}$ | 98.9 | 13332 |
| 10.6 | 121.3 | 70 | 3933 | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 118.6 | 26664 |
| -4.20 | 37.33 | 80 | 6133 | A | 23.2367 | 141 | 53323 |
| 2.7 | 66.66 | 90 | 9319 | B | 3122.45 | 164.7 | 101325 |
| 10.2 | 121.32 | 100 | 13786 | C | 5 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 44.8 |
|  |  | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |
|  |  | A | 22.1929 | bp/ ${ }^{\circ} \mathrm{C}$ | 164.54 |  |  |
|  |  | B | 3104.5 |  |  |  |  |
|  |  | C | 5.0 |  |  |  |  |

2. 

Forziati et al. 1949
Zwolinski \& Wilhoit 1971

| ebulliometry |  |  |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 81.488 | 6415 | 163.911 | 99244 | 48.82 | 1333 | 161.556 | 93326 |
| 85.857 | 7697 | 164.489 | 100733 | 62.3 | 2666 | 162.632 | 95991 |
| 89.662 | 8991 | 165.146 | 102454 | 70.85 | 4000 | 163.686 | 98659 |
| 93.131 | 10328 | 165.725 | 103987 | 77.25 | 5333 | 164.716 | 101325 |
| 96.386 | 11722 |  |  | 82.424 | 6666 |  |  |
| 100.747 | 13840 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 86.789 | 7999 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 105.716 | 16641 | A | 7.07437 | 93.949 | 10666 | A | 7.07436 |
| 110.789 | 19944 | B | 1573.267 | 99.746 | 13332 | B | 1569.622 |
| 115.498 | 23474 | C | 208.564 | 110.866 | 19998 | C | 209.578 |
| 121.765 | 28979 |  |  | 119.254 | 26664 |  |  |
| 134.464 | 43352 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 164.716 | 126.068 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | 164.716 |
| 141.618 | 53692 |  |  | 131.849 | 39997 | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ} \mathrm{mo}$ |  |
| 149.238 | 66792 |  |  | 141.387 | 53329 | at $25^{\circ} \mathrm{C}$ | 47.48 |
| 157.477 | 83752 |  |  | 149.161 | 66661 | at bp | 39.04 |
| 163.289 | 97644 |  |  | 155.772 | 79993 |  |  |



FIGURE 3.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1,3,5-trimethylbenzene.

## TABLE 3.1.1.9.3

Reported Henry's law constants of 1,3,5-trimethylbenzene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln [\mathrm{H} /(\mathrm{Pa} \mathrm{m}$
3
$3 / \mathrm{mol})]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

$$
\begin{align*}
& \log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1a}\\
& \log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \tag{2a}
\end{align*}
$$

$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

| Sanemasa et al. 1981 |  | Sanemasa et al. 1982 |  | Ashworth et al. 1988 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| vapor-liquid equilibrium |  | vapor-liquid equilibrium |  | EPICS-GC |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) | $t^{\circ} \mathrm{C}$ | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ |
| 15 | 547 | 15 | 511 | 10 | 408 |
| 25 | 929 | 25 | 887 | 15 | 466 |
| 35 | 1501 | 35 | 1365 | 20 | 477 |
| 45 | 2466 | 45 | 2394 | 25 | 682 |
|  |  |  |  | 30 | 976 |
|  |  |  |  | eq. 4 a |  |
|  |  |  |  | $\mathrm{H} /\left(\mathrm{atm} \mathrm{m}{ }^{3} / \mathrm{mol}\right)$ |  |
|  |  |  |  | A | 7.241 |
|  |  |  |  | B | 3628 |



FIGURE 3.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,3,5-trimethylbenzene.

### 3.1.1.10 n-Propylbenzene



Common Name: $n$-Propylbenzene
Synonym: 1-phenylpropane, propylbenzene
Chemical Name: $n$-propylbenzene
CAS Registry No: 103-65-1
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{2} \mathrm{CH}_{3}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -99.6 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 159.24 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.862 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$139.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 9.27 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 53.39, 59.3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
$60 \quad\left(15^{\circ} \mathrm{C}\right.$, volumetric, Fühner 1924; quoted, Chiou et al. 1982; Chiou 1985)
120 (shake flask-turbidimetric, Stearns et al. 1947)
55 (shake flask-UV, Andrews \& Keffer 1950)
120 (shake flask-UV, Klevens 1951)
60 (shake flask-GC, Hermann 1972)
70 (shake flask-GC, Krasnoshchekova \& Gubergrits 1975)
66.4 (shake flask-UV spec., Ben-Naim \& Wiff 1979)
51.9* (generator column-HPLC/UV, $15-30^{\circ} \mathrm{C}$, DeVoe et al. 1981)
51.0* (vapor saturation-UV spec., measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
47.1 (generator column.-HPLC/UV, Tewari et al. 1982a)
52.2 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)
59.5 (HPLC-k' correlation, converted from reported $\gamma_{\mathrm{w}}$, Hafkenscheid \& Tomlinson 1983a)
52.1 (generator column-HPLC/UV, Wasik et al. 1983)
45.2 (vapor saturation-UV spec., Sanemasa et al. 1984)
51.7* (generator column-HPLC/UV, measured range $10-45^{\circ} \mathrm{C}$, Owens et al. 1986)
55.0* (IUPAC recommended, temp range $15-45^{\circ} \mathrm{C}$, Shaw 1989b)
48.2* (vapor absorption technique-HPLC/UV, measured range $0.5-55^{\circ} \mathrm{C}$, Dohányosová et al. 2001)
55.0* (shake flask-UV, measured range $0-50^{\circ} \mathrm{C}$, Sawamura et al. 2001)
$\ln x=-304.679+12774.71 /(\mathrm{T} / \mathrm{K})+43.8994 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature
calorimetric and solubility data, Tsonopoulos 1999)
Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):
260* $\quad\left(13.9^{\circ} \mathrm{C}\right.$, mercury manometer, Linder 1931)
$6353^{*} \quad\left(75.646^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $75.646-160.202^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95178-1649.548 /\left(207.171+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75.6-160.2^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
667* $\quad\left(31.3^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6402 * \quad\left(75.818^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $75.818-160.239^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95094-1490.963 /\left(207.100+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75.8-160.2^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
458 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95142-1491.297 /\left(207.140+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $65-205^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
449* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95142-1491.297 /\left(207.140+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $43.33-187.87^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10424.1 /(\mathrm{T} / \mathrm{K})]+8.185880$; temp range $6.3-159.2^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-432.321 / \mathrm{T}) \times 10^{\wedge}\left(0.891023-6.89092 \times 10^{4} \cdot \mathrm{~T}+5.79948 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 280.0-635.0 K (Cox vapor pressure eq., Chao et al. 1983)

450 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.08028-1493.914 /\left(207.427+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75.2-160.24^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95142-1491.297 /\left(207.14+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $43-188^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
449 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.07438-1490.61 /(-66.029+\mathrm{T} / \mathrm{K})$; temp range $348-433 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=39.8219-3.6978 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.962 \cdot \log (\mathrm{~T} / \mathrm{K})+8.7429 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+2.6959 \mathrm{E} \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 174-638 K (Yaws 1994)
$\log (\mathrm{P} / \mathrm{kPa})=6.07625-1490.903 /[(\mathrm{T} / \mathrm{K})-66.05]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):
1062* (vapor-liquid equilibrium, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982)
1094* (EPICS-GC/FID, measured range $10-30^{\circ} \mathrm{C}$, Ashworth et al. 1988)
$\ln [\mathrm{H} /(\mathrm{atm} \cdot \mathrm{m} 3 / \mathrm{mol})]=7.835-3681 /(\mathrm{T} / \mathrm{K})$, temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
1034 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
1102 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
1175* (equilibrium headspace-GC, measured range $10-30^{\circ} \mathrm{C}$, Perlinger et al. 1993)
$902\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=4.587-1471 /(\mathrm{T} / \mathrm{K})($ van’t Hoff eq. derived from lit. data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.68 (shake flask-UV, Iwasa et al. 1965; Hansch et al. 1968; 1972)
3.57, 3.68 (Leo et al. 1971; Hansch \& Leo 1979)
3.66 (calculated-fragment const., Rekker 1977)
3.44 (shake flask-HPLC, Nahum \& Horvath 1980)
3.691* (3.701, 3.72-HPLC/UV, DeVoe et al. 1981)
3.71 (generator column-HPLC/UV both phases, Tewari et al. 1982a)
3.63 (HPLC-k' correlation, Hammers et al. 1982)
3.69 (generator column-HPLC/GC, Tewari et al. 1982b,c; Wasik et al. 1983)
3.89 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
3.69 (generator column-HPLC/UV, Wasik et al. 1983)
3.69 (generator column-RP-HPLC, Schantz \& Martire 1987)
3.71, 3.88 (RP-HPLC- $\mathrm{k}^{\prime}$ correlations, Sherblom \& Eganhouse 1988)
3.69 (recommended, Sangster 1989, 1993)
3.69 (HPLC-RT correlation, Jenke et al. 1990)
3.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ :
4.09 (calculated-measured $\gamma^{\infty}$ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
2.87 (sediment 4.02\% OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
2.83, 2.98 (RP-HPLC-k' correlation, humic acid-silica column, Szabo et al. 1990a,b)
2.81, 2.84, 2.87 (RP-HPLC-k' correlation on 3 different stationary phases, Szabo et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1 / 2}$ :
Volatilization: rate constants: $\mathrm{k}=0.037 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=19 \mathrm{~d}$ in spring at $8-16^{\circ} \mathrm{C}, \mathrm{k}=0.539 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=1.3 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{k}=0.065 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=11 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ for the periods when volatilization appears to dominate, and $\mathrm{k}=0.086 \mathrm{~d}^{-1}$, $\mathrm{t}_{1 / 2}=8.1 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in September 9-15, in marine mesocosm experiments (Wakeham et al. 1983)
Photolysis: rate constant $\mathrm{k}=6.96 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with HOin the gas (Dilling et al. 1988).
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=3.7 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(3.7 \pm 0.8) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(6.40,5.86) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysisresonance fluorescence, Ravishanakara et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=3.5 \times 10^{-9} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1.6 \mathrm{~d}$ (Mill 1982)
$\mathrm{k}_{\mathrm{OH}}=5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=6.58 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=7.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ obs. $)=5.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}-6.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=5.99 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biodegradation:
Bioconcentration

Half-Lives in the Environment:
Air: $t_{1 / 2}=2.4-24 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Danrall et al. 1976; Howard et al. 1991);
estimated lifetime $\tau=6 \mathrm{~h}$ under photochemical smog conditions in S.E. England (Brice \& Derwent 1978; Darnall et al. 1976).
Surface water: $\mathrm{t}_{1 / 2}=19 \mathrm{~d}$ in spring at $6-16^{\circ} \mathrm{C}, \mathrm{t}_{1 / 2}=1.3 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{t}_{1 / 2}=11 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ when volatilization dominates and $\mathrm{t}_{1 / 2}=8.1 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ in marine mesocosm experiments (Wakeham et al. 1983)

TABLE 3.1.1.10.1
Reported aqueous solubilities of npropylbenzene at various temperatures
1.

| Sanemasa et al. 1982 |  | DeVoe et al. 1981 |  | Owens et al. 1986 |  | Shaw 1989b (IUPAC) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| vapor saturation-UV |  | generator column-HPLC |  | generator column-HPLC |  | recommended values |  |
| $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 15 | 46.1 | 23 | 51.32 | 10 | 53.73 | 15 | 47 |
| 25 | 51 | 15 | 51.21 | 15 | 52.29 | 25 | 55 |
| 35 | 55 | 20 | 51.09 | 20 | 54.33 | 35 | 55 |
| 45 | 64.1 | 25 | 51.93 | 25 | 52.25 | 45 | 64 |
|  |  | 30 | 53.49 | 30 | 52.53 |  |  |
|  |  |  |  | 35 | 56.62 |  |  |
|  |  |  |  | 40 | 63.95 |  |  |
|  |  |  |  | 45 | 66.59 |  |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.70 \\ & 25^{\circ} \mathrm{C} \end{aligned}$ |  |  |  |  |  |  |  |

2. 

| Dohányosová et al. 2001 |  | Sawamura et al. 2001 |  |
| :---: | :---: | :---: | :---: |
| vapor absorption-HPLC/UV |  | shake flask-UV |  |
| $t^{\circ} \mathrm{C}$ | $\mathrm{s} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\prime}{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 0.5 | 46.5 | 0 | 60.2 |
| 5 | 45.8 | 5 | 57.8 |
| 15 | 44.8 | 10 | 55.96 |
| 25 | 48.2 | 15 | 54.96 |
| 35 | 52.2 | 20 | 54.5 |
| 45 | 62.4 | 25 | 54.96 |
| 55 | 74.4 | 30 | 56.2 |
|  |  | 35 | 58.4 |
| $\Delta_{\text {sol }} \mathrm{H} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=6.20$ |  | 40 | 61.3 |
| $25^{\circ} \mathrm{C}$ |  | 45 | 65.6 |
|  |  | 50 | 90.6 |



FIGURE 3.1.1.10.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $n$-propylbenzene.

TABLE 3.1.1.10.2
Reported vapor pressures of $n$-propylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  |  | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | (1a) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |  |  |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |  | (2a) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ |  |  |  | (3) |  |  |  |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ |  |  |  | (4) |  |  |  |  |  |
|  |  | Willingham | et al. 1945 | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 71 |  |
| mercury manometer |  | ebulliometry |  | summary of lit. data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -6.8 | 46.7 | 75.646 | 6353 | 6.3 | 133.3 | 75.818 | 6402 | 43.44 | 1333 |
| -0.7 | 77.3 | 80.064 | 7654 | 31.3 | 666.6 | 80.181 | 7694 | 56.79 | 2666 |
| 3.6 | 113.2 | 83.909 | 8965 | 43.4 | 1333 | 83.993 | 8993 | 65.28 | 4000 |
| 13.9 | 260 | 87.383 | 10304 | 56.8 | 2666 | 87.457 | 10332 | 71.64 | 5333 |
|  |  | 90.622 | 11696 | 71.6 | 5333 | 90.688 | 11723 | 76.784 | 6666 |
|  |  | 94.993 | 13820 | 81.1 | 7999 | 95.049 | 13844 | 81.13 | 7999 |
|  |  | 99.986 | 16621 | 94 | 13332 | 100.02 | 16636 | 88.264 | 10666 |
|  |  | 105.046 | 19924 | 113.5 | 66664 | 105.085 | 19946 | 94.046 | 13332 |
|  |  | 109.744 | 23450 | 137.7 | 53329 | 109.781 | 23557 | 105.142 | 19998 |
|  |  | 116.032 | 28955 | 159.2 | 101325 | 116.06 | 23982 | 113.542 | 26664 |
|  |  | 121.807 | 34898 |  |  | 128.794 | 43364 | 120.367 | 33331 |
|  |  | 128.764 | 43323 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -99.5 | 135.972 | 53702 | 126.163 | 39997 |
|  |  | 135.942 | 53654 |  |  | 143.625 | 66799 | 135.737 | 53329 |
|  |  | 143.598 | 66757 |  |  | 151.921 | 83753 | 143.551 | 66661 |
|  |  | 151.908 | 83718 |  |  | 157.779 | 97649 | 150.205 | 79993 |
|  |  | 157.76 | 97607 |  |  | 158.408 | 99239 | 156.031 | 93326 |
|  |  | 158.389 | 99203 |  |  | 158.991 | 100730 | 157.116 | 95992 |
|  |  | 158.972 | 100694 |  |  | 159.654 | 102465 | 158.178 | 98659 |
|  |  | 159.625 | 102386 |  |  | 160.239 | 104003 | 159.217 | 101325 |
|  |  | 160.202 | 103910 |  |  |  |  |  |  |
|  |  |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | A | 6.95094 | A | 6.95142 |
|  |  | A | 6.95178 |  |  | B | 1490.963 | B | 1491.297 |
|  |  | B | 1491548 |  |  | C | 207.1 | C | 207.14 |
|  |  | C | 207.171 |  |  |  |  |  |  |
|  |  |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 159.218 | bp/ ${ }^{\circ} \mathrm{C}$ | 159.217 |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 159.216 |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{k}$ | $\left.\mathrm{mol}^{-1}\right)=$ |
|  |  |  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 46.23 |
|  |  |  |  |  |  |  |  | at bp | 38.24 |



FIGURE 3.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-propylbenzene.

TABLE 3.1.1.10.3
Reported Henry's law constants and octanol-water partition coefficients of n-propylbenzene at various temperatures

| Henry's law constant |  |  |  |  |  | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {Ow }}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Sanemasa et al. 1982 |  | Ashworth et al. 1988 |  | Perlinger et al. 1993 |  | DeVoe et al. 1981 |  |
| vapor-liquid equilibrium |  | EPICS-GC |  | equilibrium headspace-GC |  | generator column-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m³/mol) | t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {Ow }}$ |
| 15 | 594 | 10 | 576 | 10 | 441 | 25 | 3.691 |
| 25 | 1062 | 15 | 741 | 15 | 629 | 25 | 3.701 |
| 35 | 1818 | 20 | 893 | 20 | 848 | 10 | 3.705 |
| 45 | 2754 | 25 | 1094 | 25 | 1175 | 20 | 3.735 |
|  |  | 30 | 1388 | 30 | 1550 | 25 | 3.72 |
|  |  |  |  |  |  | 30 | 3.715 |
|  |  | $\ln \mathrm{H}$ | A - B/(T/K) |  |  | 35 | 3.682 |
|  |  |  | $\left.\mathrm{m} \mathrm{m}^{3} / \mathrm{mol}\right)$ |  |  |  |  |
|  |  | A | 7.835 |  |  |  | ask-GC |
|  |  | B | 3681 |  |  | ambient | 3.734 |
|  |  |  |  |  |  | ambient | 3.718 |
|  |  |  |  |  |  | ambient | 3.711 |



FIGURE 3.1.1.10.3 Logarithm of Henry's law constant and $\mathrm{K}_{\mathrm{OA}}$ versus reciprocal temperature for $n$-propylbenzene.

### 3.1.1.11 Isopropylbenzene



Common Name: Isopropylbenzene
Synonym: cumene, 2-phenylpropane, (1-methylethyl)benzene, cumol, $i$-propylbenzene
Chemical Name: isopropylbenzene
CAS Registry No: 98-82-8
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}(\mathrm{CH})_{2}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -96.02 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 152.41 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8618 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $139.5 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 45.141, $37.53 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Riddick et al. 1986)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
7.786 (Riddick et al. 1986)
7.32 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 41.34, 46.3 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$; or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):

| 170 | (shake flask-turbidimetric, Stearns et al. 1947) |
| :--- | :--- |
| 73 | (shake flask-UV, Andrews \& Keffer, 1950) |
| $80.5^{*}$ | (shake flask-UV, measured range $25-80^{\circ} \mathrm{C}$, Glew \& Robertson 1956) |
| 53 | (shake flask-GC, McAuliffe 1963) |
| 50 | (shake flask-GC, McAuliffe 1966) |
| 50 | (shake flask-GC, Hermann 1972) |
| 65.3 | (shake flask-GC, Sutton \& Calder 1975) |
| 48.3 | (shake flask-GC, Price 1976) |
| 48.3 | (shake flask-GC, Krzyzanowska \& Szeliga 1978) |
| $61.5^{*}$ | (vapor saturation-UV, measured range $15-45^{\circ} \mathrm{C}$, Sanemasa et al. 1982) |
| $56^{*}$ | (IUPAC recommended, temp range $15-80^{\circ} \mathrm{C}$, Shaw 1989b) |

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
300* $\quad\left(13.7^{\circ} \mathrm{C}\right.$, mercury manometer, measured range $-8.2-13.7^{\circ} \mathrm{C}$, Linder 1931)
$\log (\mathrm{P} / \mathrm{mmHg})=-2175 /(\mathrm{T} / \mathrm{K})+7.991$ (isoteniscope method, temp range not specified, Kobe et al. 1941)
$6353^{*} \quad\left(70.02^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $70.02-153.367^{\circ} \mathrm{C}$, Willingham et al. 1945)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92929-1455.811 /\left(207.202+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70.0-153.4^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
$666.6^{*} \quad\left(31.3^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $6.3-159.2^{\circ} \mathrm{C}$, Stull 1947)
$6401^{*} \quad\left(70.16^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $70.16-153.4^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93958-1462.717 /\left(207.993+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70.2-153.4^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

621 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Hine \& Mookerjee 1975)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93666-1460.793 /\left(207.777+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $60-200^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
609 (interpolated, Glew \& Robertson 1956)
611* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93666-1460.793 /\left(207.777+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $38.29-180.67^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10335.3 /(\mathrm{T} / \mathrm{K})]+8.231760$; temp range $2.9-152.4^{\circ} \mathrm{C}$ (Antoine eq., Weast $\left.1972-73\right)$
$\log (\mathrm{P} / \mathrm{atm})=(1-425.438 / \mathrm{T}) \times 10^{\wedge}\left(0.877964-7.34971 \times 10^{4} \cdot \mathrm{~T}+6.06942 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range
264.95-630.0 K (Cox vapor pressure eq., Chao et al. 1983)

610 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.0571-1457.715 /\left(207.415+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70.02-153.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.06528-1464.366 /\left(208.235+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $56.39-151.69^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Dreyer et al. 1955, Boublik et al. 1984)
610 (selected lit., Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.06588-1464.17 /\left(208.207+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Riddick et al. 1986) $\log (\mathrm{P} / \mathrm{mmHg})=6.93666-1460.793 /\left(207.78+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $39-181^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
605 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.05949-1459.975 /(-65.942+\mathrm{T} / \mathrm{K})$; temp range $339-433 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-0.9234-2.9558 \times 10^{3} /(\mathrm{T} / \mathrm{K})+7.1685 \cdot \log (\mathrm{~T} / \mathrm{K})-2.5369 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.4858 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $177-631 \mathrm{~K}$ (Yaws 1994)
$\log \mathrm{P} / \mathrm{kPa}=6.06149-1460.793 /[(\mathrm{T} / \mathrm{K})-65.373]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):

| 1469 | $($ calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |
| :--- | :--- |
| $1323^{*}$ | $\left(28^{\circ} \mathrm{C}\right.$, EPICS-GC, measured range $28-46.1^{\circ} \mathrm{C}$, Hansen et al. 1993) |
| $\ln \left[\mathrm{H} /\left(\mathrm{kPa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=-3269 /(\mathrm{T} / \mathrm{K})+11.0 ;$ temp range $28-46.1^{\circ} \mathrm{C}$ (EPICS-GC, Hansen et al. 1993) |  |
| 1126 | (infinite activity coeff. $\gamma^{\circ}$ in water determined by inert gas stripping-GC, Li et al. 1993) |
| 960 | $\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996) |
| 902 | $\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 2001) |
| $\log \mathrm{K}_{\mathrm{AW}}=3.774-1256 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001) |  |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.43 (calculated- $\pi$ substituent constant, Hansch et al. 1968)
3.66 (Leo et al. 1971; Hansch \& Leo 1979)
3.63 (shake flask-GC, Chiou et al. 1977, 1982)
3.51 (headspace GC, Hutchinson et al. 1980)
3.52 (HPLC-k' correlation, Hanai et al. 1981)
3.52 (HPLC-k' correlation, D’Amboise \& Hanai 1982)
3.40 (HPLC-k' correlation, Miyake \& Terada 1982)
3.89, 4.07 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
3.66 (recommended, Sangster 1989, 1993)
3.82 (from measured activity coeff., Tse et al. 1994)
3.66 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ :
3.98 (calculated-measured $\gamma^{\infty}$ in pure octanol of Tewari et al. 1982, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
1.55 (goldfish, Ogata et al. 1984)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: $\mathrm{t}_{1 / 2}=5.7 \mathrm{~h}$ from water depth of 1 m (calculated, Mackay \& Leinonen 1975).
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(3.7 \pm 0.8) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=3.7 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=2.4-24 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(7.79 \pm 0.40) \times 10^{-12} \mathrm{~cm}^{3}$ molecule $^{-1} \mathrm{~s}^{-1}$ at 200 torr He and 298 K (flash photolysis-resonance fluorescence, Ravishanakara et al. 1978)
$\mathrm{k}_{\mathrm{OH}}=4.6 \times 10^{-1} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1.2 \mathrm{~d}$ (Mill 1982)
$\mathrm{k}=(11 \pm 3) \mathrm{M}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone in water using $100 \mathrm{mM} t-\mathrm{BuOH}$ as scavenger at pH 2.0 and $20-23^{\circ} \mathrm{C}$ (Hoigné \& Bader 1983)
$\mathrm{k}_{\mathrm{OH}}=6.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=6.25 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=7.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}\left(\right.$ obs.) $=6.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}=6.5 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=4.69 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biodegradation:
Bioconcentration

Half-Lives in the Environment:
Air: $t_{1 / 2}=2.4-24 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);
estimated lifetime $\tau=6 \mathrm{~h}$ under photochemical smog conditions in S.E. England (Brice \& Derwent 1978) and (Darnall et al. 1976).
Surface Water: $\mathrm{t}_{1 / 2}=5.79 \mathrm{~h}$, calculated half-life based on evaporative loss at $25^{\circ} \mathrm{C}$ and 1 m depth of water (Mackay \& Leinonen 1975).

TABLE 3.1.1.11.1
Reported aqueous solubilities and Henry's law constants of isopropylbenzene at various temperatures

| Aqueous solubility |  |  |  |  |  | Henry's law constant Hansen et al. 1993 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Glew \& Robertson 1956 |  | Sanemasa et al. 1982 |  | Shaw 1989b (IUPAC) |  |  |  |
| shake flask-UV spec. |  | vapor equilibrium-UV spec. |  | recommended values |  | EPICS-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 24.936 | 80.47 | 15 | 59.5 | 15 | 60 | 28 | 1323 |
| 29.984 | 82.91 | 25 | 61.5 | 25 | 56 | 36 | 1547 |
| 34.918 | 85.64 | 35 | 68.7 | 30 | 74 | 46.1 | 2422 |
| 39.958 | 89.79 | 45 | 77.5 | 40 | 82 |  |  |
| 44.905 | 94.57 |  |  | 50 | 90 | $\ln \mathrm{H}$ | $\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| 49.902 | 100.4 | $\Delta \mathrm{H}_{\text {sol }}$ | $)=5.10$ | 60 | 120 |  | $\mathrm{Pa} \mathrm{m} / \mathrm{mol})$ |
| 54.916 | 106.9 |  |  | 70 | 140 | A | 11 |
| 59.983 | 115 |  |  | 80 | 160 | B | 3299 |
| 65.165 | 124.4 |  |  |  |  |  |  |
| 70.32 | 135.6 |  |  |  |  |  |  |
| $75.097$ | 147.3 |  |  |  |  |  |  |
| 80.209 | 161.7 |  |  |  |  |  |  |
| $\begin{gathered} \Delta \mathrm{H}_{\text {sol }}\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=3.57 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  |  |  |  |  |  |  |



FIGURE 3.1.1.11.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for isopropylbenzene.

TABLE 3.1.1.11.2
Reported vapor pressures of isopropylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| Linder 1931 |  | Willingham et al. 1945 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Hg manometer |  | ebulliometry |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -8.2 | 57.3 | 70.02 | 6353 | 70.16 | 6401 | 36.29 | 1333 |
| 1.3 | 124 | 74.365 | 7654 | 74.47 | 7693 | 51.43 | 2666 |
| 13.7 | 300 | 78.155 | 8965 | 78.23 | 8993 | 59.79 | 4000 |
|  |  | 81.579 | 10304 | 81.64 | 10331 | 66.06 | 5333 |
|  |  | 84.768 | 11696 | 89.11 | 11722 | 71.123 | 6666 |
|  |  | 89.077 | 13820 | 94.01 | 13843 | 75.407 | 7999 |
|  |  | 93.991 | 16621 | 99 | 16636 | 82.433 | 10666 |
|  |  | 98.975 | 19924 | 103.64 | 19946 | 88.13 | 13332 |
| Stull 1947 |  | 103.604 | 23450 | 109.82 | 23477 | 99.076 | 19998 |
| summary of lit. data |  | 109.802 | 28995 | 115.52 | 28980 | 107.346 | 26664 |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | 115.495 | 34898 | 12.38 | 34928 | 114.076 | 33331 |
| 6.3 | 133 | 122.353 | 43323 | 129.46 | 43363 | 119.789 | 39997 |
| 31.3 | 666.6 | 129.433 | 53654 | 137.01 | 53701 | 129.23 | 53329 |
| 43.4 | 1333 | 136.983 | 66757 | 145.19 | 66799 | 136.937 | 66661 |
| 56.8 | 2666 | 145.176 | 83718 | 150.97 | 83752 | 143.501 | 79993 |
| 71.6 | 5333 | 150.956 | 97607 | 151.59 | 97649 | 149.249 | 93326 |
| 81.1 | 7999 | 151.576 | 99203 | 152.17 | 100730 | 150.319 | 95992 |
| 94 | 13332 | 152.152 | 100694 | 152.82 | 102465 | 151.367 | 98659 |
| 113.5 | 26664 | 152.798 | 102386 | 153.4 | 104003 | 152.392 | 101325 |
| 137.7 | 53329 | 153.367 | 103910 |  |  |  |  |
| 159.2 | 101325 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | A | 6.93958 | A | 6.93666 |
|  | -99.5 | A | 6.92929 | B | 1462.717 | B | 1460.793 |
|  |  | B | 1455.81 | C | 207.993 | C | 207.777 |
|  |  | C | 207.202 |  | 152.392 |  |  |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 152.393 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ |  | bp/ ${ }^{\circ} \mathrm{C}$ | 152.392 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 45.14 |
|  |  |  |  |  |  | at bp | 37.53 |



FIGURE 3.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for isopropylbenzene.

### 3.1.1.12 1-Ethyl-2-methylbenzene (o-Ethyltoluene)



Common Name: 1-Ethyl-2-methylbenzene
Synonym: 2-ethyltoluene, o-ethyltoluene
Chemical Name: 1-ethyl-2-methylbenzene, 1-methyl-2-ethylbenzene
CAS Registry No: 611-14-3
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}_{3} \mathrm{C}_{2} \mathrm{H}_{5}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-79.83 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 165.2 (Weast 1982-83; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8807 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $136.5 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

| 40.0 | (estimated from nomograph, Kabadi \& Danner 1979) |
| :--- | :--- |
| 93.05 | (shake flask-GC, Mackay \& Shiu 1981) |
| 74.6 | (generator column-HPLC/UV, Tewari et al. 1982c) |

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$133.3^{*} \quad\left(9.4^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6417 * \quad\left(81.146^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $81.146-157.825^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00314-1535.374 /\left(207.300+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $81.1-166.2^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
336 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00314-1535.374 /\left(207.3+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70-215^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
330* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00314-1535.374 /\left(207.300+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $48.46-193.89^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10448.8 /(\mathrm{T} / \mathrm{K})]+8.141032$; temp range $9.4-165.2^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-438.357 / \mathrm{T}) \times 10^{\wedge}\left(0.863837-6.34917 \times 10^{4} \cdot \mathrm{~T}+5.19164 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 285.0-645.0 K (Cox vapor pressure eq., Chao et al. 1983)

328 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.11997-1529.684 /\left(206.648+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $81.146-166.2^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data Forziati et al. 1949, Boublik et al. 1984)
330 (extrapolated-Antoine eq, Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.00314-1535.374 /\left(207.30+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $48-194^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1129-1532.449 /(-66.123+\mathrm{T} / \mathrm{K})$; temp range $353-443 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=15.1142-2.9821 \times 10^{3} /(\mathrm{T} / \mathrm{K})-1.2619 \cdot \log (\mathrm{~T} / \mathrm{K})-6.3248 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+3.5155 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 192-651 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
565 (EPICS-GC/FID, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \mathrm{m} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=5.557-3179 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS measurements, Ashworth et al. 1988)
426 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
$512\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
3.63 (headspace GC, Hutchinson et al. 1980)
3.53 (generator column-HPLC/UV, DeVoe et al.1981; Tewari et al. 1982a)
3.78, 3.95 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
3.53 (recommended, Sangster 1989, 1993)
3.53 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(8.2 \pm 1.6) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=8.2 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with half-life of $0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=12.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=12.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=12.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990) $\mathrm{k}_{\mathrm{OH}}($ calc $)=17.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration
Half-Lives in the Environment:
Air: $t_{1 / 2}=0.24-2.4 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991);
summer daylight lifetime $\tau=11 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991).
Surface water: $t_{1 / 2}=0.5 \mathrm{~d}$ in surface water in case of a first order reduction process may be assumed (estimated, Zoeteman et al. 1980).

TABLE 3.1.1.12.1
Reported vapor pressures of o-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |


| Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | ebulliometry |  | selected values |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |  |  |
| 9.4 | 133.3 | 81.146 | 6417 | 48.46 | 1333 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 34.8 | 666.6 | 85.618 | 7697 | 61.96 | 2666 | A | 7.00314 |
| 47.6 | 1333 | 89.448 | 8993 | 70.54 | 4000 | B | 1535.374 |
| 61.2 | 2666 | 92.949 | 10323 | 76.97 | 5333 | C | 207.3 |
| 76.4 | 5333 | 96.2 | 11720 | 82.165 | 6666 | bp/ ${ }^{\circ} \mathrm{C}$ | 165.153 |
| 86 | 7999 | 100.584 | 13840 | 86.552 | 7999 |  | $\left(\mathrm{mol}^{-1}\right)=$ |
| 99 | 13332 | 105.598 | 16641 | 93.751 | 10666 | at $25^{\circ} \mathrm{C}$ | 47.7 |
| 119 | 26664 | 110.711 | 19944 | 99.582 | 13332 | at bp | 38.87 |
| 141.4 | 53329 | 115.436 | 23473 | 110.777 | 19998 |  |  |
| 165.1 | 101325 | 121.762 | 28978 | 119.29 | 26664 |  |  |
|  |  | 127.574 | 34920 | 126.1 | 33331 |  |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -104.7 | 134.57 | 43351 | 131.933 | 39997 |  |  |
|  |  | 141.792 | 53693 | 141.563 | 53329 |  |  |
|  |  | 149.582 | 66792 | 149.418 | 66661 |  |  |
|  |  | 157.825 | 83749 | 156.103 | 79993 |  |  |
|  |  |  |  | 161.954 | 93326 |  |  |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 164.044 | 95992 |  |  |
|  |  | A | 7.00314 | 164.11 | 98659 |  |  |
|  |  | B | 1535.374 | 165.534 | 101325 |  |  |
|  |  | C | 207.3 |  |  |  |  |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 165.153 |  |  |  |  |



FIGURE 3.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-2-methylbenzene (oethyltoluene).

### 3.1.1.13 1-Ethyl-3-methylbenzene (m-Ethyltoluene)



Common Name: 1-Ethyl-3-methylbenzene
Synonym: 3-ethyltoluene, m-ethyl toluene
Chemical Name: 1-ethyl-3-methylbenzene, 1-methyl-3-ethylbenzene
CAS Registry No: 620-14-4
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}_{3} \mathrm{C}_{2} \mathrm{H}_{5}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): - $95.6 \quad$ (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
161.3 (Forziati et al. 1949, Weast 1982-83; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.8645 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$139.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$666.6^{*} \quad\left(32.3^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $7.2-161.3^{\circ} \mathrm{C}$, Stull 1947)
3066* $\quad\left(62.1^{\circ} \mathrm{C}\right.$, mercury manometer, measured range $62.1-160.3^{\circ} \mathrm{C}$, Buck et al. 1949)
$6417^{*} \quad\left(78.105^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $78.105-154.053^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01582-1529.784 /\left(208.509+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $78.1-162.3^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
399 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01582-1529.184 /\left(208.509+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $65-210^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
391* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01582-1529.184 /\left(208.509+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $45.68-189.74^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10416.6 /(\mathrm{T} / \mathrm{K})]+8.152199$; temp range $7.2-161.3^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-434.538 / \mathrm{T}) \times 10^{\wedge}\left(0.861399-6.30303 \times 10^{4} \cdot \mathrm{~T}+5.19848 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range
280.0-635.0 K (Cox vapor pressure eq., Chao et al. 1983)

394 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.12947-1531.584 /\left(209.417+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $78.3-163^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
391 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01582-1529.184 /\left(208.51+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $46-190^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
391 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.13801-1527.983 /(-64.715+\mathrm{T} / \mathrm{K})$; temp range $348-438 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=39.8909-3.6042 \times 10^{3} /(\mathrm{T} / \mathrm{K})-11.466 \cdot \log (\mathrm{~T} / \mathrm{K})+3.5274 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+7.3492 \times 10^{-14} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 178-637 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.88, 4.07 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
3.98 (lit. average value, Sangster 1993)
3.88 (quoted from Sherblom \& Eganhouse 1988; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
2.42 (aquifer material with $\mathrm{f}_{\mathrm{OC}}$ of 0.006 and measured partition coeff. $\mathrm{K}_{\mathrm{P}}=1.58 \mathrm{~mL} / \mathrm{g}$., Abdul et al. 1990)

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(11.7 \pm 2.3) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm \mathrm{K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=11.7 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with estimated $\mathrm{t}_{1 / 2} \sim 0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=(21.3 \pm 1.1) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate method, Ohta \& Ohyama 1985; Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=1.92 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=20.93 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:
Air: $t_{1 / 2}=0.24-2.4 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al 1976; Howard et al. 1991);
summer daylight lifetime $\tau=7.2 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991).

TABLE 3.1.1.13.1
Reported vapor pressures of $m$-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations



FIGURE 3.1.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for 1 -ethyl-3-methylbenzene ( $m$-ethyltoluene).

### 3.1.1.14 1-Ethyl-4-methylbenzene ( $p$-Ethyltoluene)



Common Name: 1-Ethyl-4-methylbenzene
Synonym: 4-ethyltoluene, p-ethyl toluene
Chemical Name: 1-ethyl-4-methylbenzene, 1-methyl-4-ethylbenzene
CAS Registry No: 622-96-8
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{12}, \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}_{3} \mathrm{C}_{2} \mathrm{H}_{5}$
Molecular Weight: 120.191
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-62.35 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
162 (Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.8614 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$139.5\left(20^{\circ} \mathrm{C}\right.$, calculated -density, Stephenson \& Malanowski 1987)
162.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
40.0 (estimated from nomograph, Kabadi \& Danner 1979)
94.85 (shake flask-GC, Mackay \& Shiu 1981)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$666.6^{*} \quad\left(32.7^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $7.6-162^{\circ} \mathrm{C}$, Stull 1947)
$3840^{*} \quad\left(66.8^{\circ} \mathrm{C}\right.$, mercury manometer, measured range $66.8-161.1^{\circ} \mathrm{C}$, Buck et al. 1949)
6417* $\quad\left(78.396^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $78.396-154.684^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99801-1527.113 /\left(208.921+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $78.3-163.0^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
402 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99802-1527.113 /\left(208.921+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $65-210^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
393* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99802-1527.113 /\left(208.921+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $45.68-190.64^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10461.1 /(\mathrm{T} / \mathrm{K})]+8.175267$; temp range $7.6-162^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-345.228 / \mathrm{T}) \times 10^{\wedge}\left(0.856105-6.18307 \times 10^{4} \cdot \mathrm{~T}+5.08568 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 280.0-635.0 K (Cox vapor pressure eq., Chao et al. 1983)

393 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99802-1527.113 /\left(208.92+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $46-191^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.11098-1519.486 /(-65.035+\mathrm{T} / \mathrm{K})$; temp range $349-442 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=46.9026-3,8382 \times 10^{3} /(\mathrm{T} / \mathrm{K})-14.154 \cdot \log (\mathrm{~T} / \mathrm{K})+4.9305 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-1.3901 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 211-640 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 498 | (calculated-P/C, Mackay \& Shiu 1981, Eastcott et al. 1988) |
| :--- | :--- |
| 498 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
3.63 (headspace GC, Hutchinson et al. 1980)
3.90, 4.09 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
3.63 (recommended, Sangster 1989, 1993)
3.90 (quoted from Sherblom \& Eganhouse 1988, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\text {OH }}=(7.8 \pm 1.6) \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ at $305 \pm 2 \mathrm{~K}$ (relative rate method, Lloyd et al. 1976)
$\mathrm{k}_{\mathrm{OH}}=7.8 \times 10^{9} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$ (Darnall et al. 1976)
$\mathrm{k}_{\text {OH }}=12.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule $\mathrm{e}^{-1} \mathrm{~s}^{-1}$ and residence time of 0.9 d , loss of $67 \%$ in one day or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
$\mathrm{k}_{\mathrm{OH}}=11.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=12.8 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (relative rate method, Ohta \& Ohyama 1985)
$\mathrm{k}_{\mathrm{OH}}=12.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=21.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.24-2.4 \mathrm{~h}$, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976) residence time of 0.9 d , loss of $67 \%$ in 1 d or 12 sunlit hours at 300 K in urban environments (Singh et al. 1981)
summer daylight lifetime $\tau=11 \mathrm{~h}$ due to reaction with OH radical (Altshuller 1991).

TABLE 3.1.1.14.1
Reported vapor pressures of $p$-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | (1) (2) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | (1a) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $P=A-B /(C+$ |  |  |  | $\cdots$ |  |  |
| $\begin{equation*} \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{~T} / \mathrm{K}) \tag{4} \end{equation*}$ |  |  |  |  |  |  |  |
| Stull 1947 |  | Forziati et al. 1949 |  | Buck et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| summary of literature data |  | ebulliometry |  | mercury manometer |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 7.6 | 133.3 | 78.396 | 6417 | 66.8 | 3840 | 45.68 | 1333 |
| 32.7 | 666.6 | 82.701 | 7657 | 77.4 | 6106 | 59.14 | 2666 |
| 44.9 | 1333 | 86.523 | 8993 | 79.4 | 6586 | 67.68 | 4000 |
| 58.5 | 2666 | 89.988 | 10328 | 83.5 | 7999 | 74.09 | 5333 |
| 73.6 | 5333 | 93.252 | 11720 | 87.9 | 9466 | 79.265 | 6666 |
| 83.2 | 7999 | 97.63 | 13840 | 90.2 | 10399 | 83.637 | 7999 |
| 96.3 | 13332 | 102.619 | 16641 | 94 | 11999 | 90.811 | 10666 |
| 116.1 | 26664 | 107.71 | 19944 | 105.8 | 18638 | 96.623 | 13332 |
| 136.4 | 53329 | 112.422 | 23474 | 122.7 | 33197 | 107.781 | 19998 |
| 162 | 101325 | 118.727 | 28978 | 131.7 | 44130 | 116.205 | 26664 |
|  |  | 131.499 | 43351 | 136.9 | 51329 | 123.054 | 33331 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | - | 139.701 | 53693 | 144.2 | 63595 | 128.869 | 39997 |
|  |  | 146.368 | 66792 | 152.5 | 79727 | 138.469 | 53329 |
|  |  | 154.684 | 83750 | 161.1 | 100792 | 146.3 | 66661 |
|  |  |  |  |  |  | 152.965 | 79993 |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 158.799 | 93326 |
|  |  | A | 6.99801 | A | 21.27 | 159.885 | 95992 |
|  |  | B | 1527.113 | B | 2939 | 160.948 | 98659 |
|  |  | C | 208.921 | C | 4.406 | 161.989 | 101325 |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 161.989 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 6.99802 |
|  |  |  |  |  |  | B | 1527.113 |
|  |  |  |  |  |  | C | 208.921 |
|  |  |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 161.989 |
|  |  |  |  |  |  |  | $\mathrm{kJ} \mathrm{mol}^{-1}$ ) $=$ |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 46.61 |
|  |  |  |  |  |  | at bp | 38.41 |



FIGURE 3.1.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for 1 -ethyl-4-methylbenzene ( $p$ ethyltoluene).

### 3.1.1.15 1-Isopropyl-4-methylbenzene (p-Cymene)



Common Name: 1-Isopropyl-4-methylbenzene
Synonym: p-cymene, p-isopropyltoluene, 1-methyl-4-isopropylbenzene
Chemical Name: 1-isopropyl-4-methylbenzene
CAS Registry No: 99-87-6
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{CH}_{3} \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-67.94 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
177.1 (Weast 1982-83; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8573 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$156.6 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
9.66 (Dreisbach 1955)
9.67 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
47.33, 46.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

| 34.15 | (residue volume method, Booth \& Everson 1948) |
| :--- | :--- |
| 23.35 | (shake flask-LSC, Banerjee et al. 1980) |
| $50.7 \pm 2.3$ | (shake flask-HPLC/UV, Lun et al. 1997) |

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
90.7* $\quad\left(13.3^{\circ} \mathrm{C}\right.$, mercury manometer, Linder 1931)
$\log (\mathrm{P} / \mathrm{mmHg})=8.063-10670 /(\mathrm{T} / \mathrm{K})($ isoteniscope method, measured range not specified, Kobe et al. 1941)
133.3* ( $19^{\circ} \mathrm{C}$, summary of literature data, Stull 1947)

212 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9260-1538.00 /\left(203.10+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $80-215^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

12026* ( $107.04^{\circ} \mathrm{C}$, ebulliometry, measured range 107.04-178.42 ${ }^{\circ} \mathrm{C}$, McDonald et al. 1959)
204* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9237-1537.06 /\left(203.05+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $56.4-207.1^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{atm})=(1-450.311 / \mathrm{T}) \times 10^{\wedge}\left(0.875129-6.86627 \times 10^{4} \cdot \mathrm{~T}+5.61507 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range
290.0-650.0 K (Cox vapor pressure eq., Chao et al. 1983)
$\log (\mathrm{P} / \mathrm{mmHg})=7.05074-1608.91 /\left(208.72+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $107-178^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
194 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16214-1599.29 /(-65.492+\mathrm{T} / \mathrm{K})$; temp range $380-452 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-5.5137-3.0256 \times 10^{3} /(\mathrm{T} / \mathrm{K})+8.9840 \cdot \log (\mathrm{~T} / \mathrm{K})-2.5597 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.3823 \times 10^{-5} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 205-653 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

$$
800 \quad \text { (calculated-P/C, Mackay \& Shiu 1981) }
$$

942 (computed-expert system SPARC, Kollig 1995)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.10 (shake flask-LSC, Banerjee et al. 1980)
4.14 (calculated-UNIFAC activity coeff., Arbuckle 1983)
3.45 (calculated-UNIFAC activity coeff., Banerjee \& Howard 1988)
4.10 (recommended, Sangster 1989)
4.10 (recommended, Hansch et al. 1995)
4.0 (computed-expert system SPARC, Kollig 1995)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
3.70 (computed- $\mathrm{K}_{\mathrm{ow}}$, Kollig 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: rate constant of $1.68 \times 10^{-2} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with $\mathrm{HO} \cdot$ in the gas (Dilling et al. 1988).
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=0.92 \times 10^{11} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ at room temp. (estimated from structurally similar $p$-ethyltoluene, Winer et al. 1976)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=1.50 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (SAR, Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}=1.53 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Dilling et al. 1988)
$\mathrm{k}_{\mathrm{OH}}=(1.51 \pm 0.41) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a tropospheric lifetime $\tau=1.0-1.4 \mathrm{~d} ; \mathrm{k}_{\mathrm{NO} 3}=$ $(9.9 \pm 1.6) \times 10^{-16} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a tropospheric lifetime $\tau=1.3 \mathrm{yr}$ and a calculated tropospheric lifetime $\tau>330 \mathrm{~d}$ due to reaction with $\mathrm{O}_{3}$ at $295 \pm 2 \mathrm{~K}$ (relative rate method, Corchnoy \& Atkinson 1990)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration
Half-Lives in the Environment:
Air: calculated tropospheric lifetimes of 1.0 d , $>330 \mathrm{~d}$ and 1.3 yr due to reactions with OH radical, $\mathrm{O}_{3}$ and $\mathrm{NO}_{3}$ radical, respectively (Corchnoy \& Atkinson 1990)

TABLE 3.1.1.15.1
Reported vapor pressures of $p$-cymene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | (1) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | (1a) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}$ | $1{ }^{\circ} \mathrm{C}$ ) | (2) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /($ | $\left.+t^{\circ} \mathrm{C}\right)$ | (2a) |
|  | $\log P=A-B /(C$ | T/K) | (3) |  |  |  |  |
|  | $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T}$ | - C•log (T/K) | (4) |  |  |  |  |
| Linder 1931 |  | Stull 1947 |  | McDonald et al. 1959 |  | Zwolinski \& Wilhoit 1971 |  |
| mercury manometer |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -3.5 | 18.67 | 19 | 133.3 | 107.04 | 12026 | 56.4 | 1333 |
| -5.3 | 18.67 | 44.6 | 666.6 | 128.24 | 25189 | 70.3 | 2666 |
| 0 | 30.66 | 57.6 | 1333 | 151.9 | 51745 | 79.2 | 4000 |
| 0.8 | 33.33 | 71.5 | 2666 | 175.35 | 96965 | 85.8 | 5333 |
| 13.3 | 90.66 | 87 | 5333 | 176.46 | 99792 | 91.1 | 6666 |
|  |  | 96.8 | 7999 | 177.36 | 101949 | 95.7 | 7999 |
|  |  | 110.1 | 13332 | 178.42 | 104553 | 103.1 | 10666 |
|  |  | 130 | 26664 |  |  | 109.3 | 13332 |
|  |  | 151.8 | 53329 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 120.7 | 19998 |
|  |  | 175 | 101325 | A | 7.03724 | 129.5 | 26664 |
|  |  |  |  | B | 1599.29 | 136.5 | 33331 |
|  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | C | 207.659 | 142.6 | 39997 |
|  |  |  |  |  |  | 152.6 | 53329 |
|  |  |  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -67.98 | 108 | 66661 |
|  | Kobe et al. 1941 |  |  |  |  | 167.7 | 79993 |
| isoteniscope method |  |  |  |  |  | 173.8 | 93326 |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |  |  |  |  | 174.94 | 95992 |
| data presented by |  |  |  |  |  | 176.05 | 98659 |
|  |  |  |  |  |  | 177.13 | 101325 |
| eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |  |  |
| A | 8.063 |  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| B | 2332 |  |  |  |  | A | 6.9237 |
|  |  |  |  |  |  | B | 1537.06 |
| bp/ $/{ }^{\circ} \mathrm{C}$ | 176.8 |  |  |  |  | C | 203.05 |
| $\Delta \mathrm{H}_{\mathrm{v}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=44.64$ |  |  |  |  |  |  |  |
|  |  |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 177.13 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 50.29 |
|  |  |  |  |  |  | at bp | 38.16 |



FIGURE 3.1.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for 1-isopropyl-4-methylbenzene (p-cymene).

### 3.1.1.16 $n$-Butylbenzene



Common Name: $n$-Butylbenzene
Synonym: butylbenzene
Chemical Name: n-butylbenzene
CAS Registry No: 104-51-8
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{3} \mathrm{CH}_{3}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -87.85 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 183.31 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.8601 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$156.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
10.98 (Dreisbach 1955)
11.22 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
60.56, 66.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$; *data at other temperatures are tabulated at end of section):
12.6 (shake flask-UV, Andrews \& Keefer 1950)
50.5 (shake flask-UV, Klevens 1950)
15.4 (estimated, Deno \& Berkheimer 1960)
17.7 (shake flask-GC/ECD, Massaldi \& King 1973)
11.8 (shake flask-GC, Sutton \& Calder 1975)
12.6 (shake flask-GC, Mackay \& Shiu 1981)
13.83 (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982)
13.8 (generator column-HPLC/UV, Wasik et al. 1983)
13.76* (generator column-HPLC/UV, measured range $7-45^{\circ} \mathrm{C}$, Owens et al. 1986)
15.0 (IUPAC recommended, Shaw 1989b)
$16.7^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, equilibrium flow cell-GC, measured range $30-100^{\circ} \mathrm{C}$, Chen \& Wagner 1994c)
$\ln x=-43.2390-5720.35 /(\mathrm{T} / \mathrm{K})-1.221 \times 10^{-4} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
12.25* (vapor absorption technique-HPLC/UV, measured range $0.5-55^{\circ} \mathrm{C}$, Dohányosová et al. 2001)
$\ln x=-346.295+14524.83 /(\mathrm{T} / \mathrm{K})+49.9130 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations; * data at other temperatures are tabulated at end of section):
64* $\quad\left(12.2^{\circ} \mathrm{C}\right.$, mercury manometer, Linder 1931)
133.3* $\left(22.7^{\circ} \mathrm{C}\right.$, summary of literature data, Stull 1947)
$6415^{*} \quad\left(96.233^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $96.233-184.329^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98318-1577.965 /\left(201.378+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $96.2-184.2^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
145 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98317-1577.965 /\left(201.378+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $85-220^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

137* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98317-1577.965 /\left(201.378+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $62.36-213.1^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 11052.1 /(\mathrm{T} / \mathrm{K})]+8.194170$; temp range $22.7-183.1^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-456.368 / \mathrm{T}) \times 10^{\wedge}\left(0.889482-7.01171 \times 10^{4} \cdot \mathrm{~T}+5.65027 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 295.0-660.0 K (Cox vapor pressure eq., Chao et al. 1983)

138, 147 (extrapolated-Antoine equations, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.11624-1583.708 /\left(202.013+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $96.2-184.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.22353-1660.274 /\left(210.314+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $101.3-181.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.98317-1577.965 /\left(201.378+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $62-213^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.09809-1571.648 /(-72.413+\mathrm{T} / \mathrm{K})$; temp range: $369-463 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$110 \quad\left(20.51^{\circ} \mathrm{C}\right.$, static method, measured range 243.8-403.14 K, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{kPa})=6.41845-1779.018 /\left(220.982+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $243.8-403.14 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=49.9687-4.3981 \times 10^{3} /(\mathrm{T} / \mathrm{K})-14.352 \cdot \log (\mathrm{~T} / \mathrm{K})+4.2054 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.4379 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $185-661 \mathrm{~K}$ (Yaws 1994)
$107 \quad\left(20.16^{\circ} \mathrm{C}\right.$, static method, measured range $253.76-418.04 \mathrm{~K}$, Mokbel et al. 1998)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C} ; *$ data at other temperatures are tabulated at end of section):
1300 (calculated-P/C, Mackay \& Shiu 1981)
1332 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
1502 (infinite activity coeff. $\gamma^{\infty}$ in water determined by inert gas stripping-GC, Li et al. 1993)
1692* (equilibrium headspace-GC, Perlinger et al. 1993)
1357.8 (modified EPICS method-GC, Ryu \& Park 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.26 (Hansch \& Leo 1979)
4.19 (calculated-fragment const., Rekker 1977)
3.86 (headspace GC, Hutchinson et al. 1980)
4.26 (HPLC-k' correlation, Hammers et al. 1982)
4.28 (generator column-HPLC/UV, Tewari et al. 1982c)
4.21 (HPLC methods, Harnisch et al. 1983)
4.28 (generator column-HPLC/UV, Wasik et al. 1983)
4.29 (generator column-RP-LC, Schantz \& Martire 1987)
4.26, 4.50 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.26 (recommended, Sangster 1989, 1993)
4.377 (shake flask/slow stirring-GC, De Brujin et al. 1989)
4.38 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.39 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach \& Westall 1981)
3.40 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
3.52 (RP-HPLC- $k^{\prime}$ correlation, cyanopropyl column, Hodson \& Williams 1988)
3.15, 3.32 (RP-HPLC-k' correlation, Szabo et al. 1990a,b)
3.35, 3.38, 3.39 (RP-HPLC-k' correlation on different stationary phases, Szabo et al. 1995)

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 3.1.1.16.1
Reported aqueous solubilities and Henry's law constants of nbutylbenzene at various temperatures

| Aqueous solubility |  |  |  |  | Henry's law constant <br> Perlinger et al. 1993 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Owens et al. 1986 | Chen \& Wagner 1994c |  | Dohány | al. 2001 |  |  |
| generator column-HPLC | equilib | cell-GC | vapor | LC/UV | equ | headspace-GC |
| $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| $7 \quad 13.34$ | 30 | 16.7 | 0.5 | 11.5 | 10 | 543 |
| $10 \quad 12.98$ | 40 | 17.82 | 5 | 11.5 | 15 | 828 |
| 12.5 13.14 | 50 | 20.3 | 15 | 11.3 | 20 | 1115 |
| $15 \quad 12.97$ | 60 | 26.9 | 25 | 12.25 | 25 | 1692 |
| 17.5 - 13.14 | 70 | 32.06 | 35 | 14.5 | 30 | 2168 |
| $20 \quad 13.66$ | 80 | 47.72 | 45 | 17.6 |  |  |
| $25 \quad 13.76$ | 90 | 61.14 | 55 | 21.2 |  |  |
| $30 \quad 14.58$ | 100 | 83.5 |  |  |  |  |
| $35 \quad 15.4$ | $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=1.29 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=1.29$ |  |  |  |
| $40 \quad 1763$ |  |  |  |  |  |  |
| $45 \quad 20.21$ |  |  |  |  |  |  |
| $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=6.60 \\ \text { at } 25^{\circ} \mathrm{C} \end{gathered}$ |  |  |  |  |  |  |



FIGURE 3.1.1.16.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for $n$-butylbenzene.

TABLE 3.1.1.16.2
Reported vapor pressures of $n$-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | (1) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | (1a) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | A - B//C | $\left./^{\circ} \mathrm{C}\right)$ | (2) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B}$ | $\left.+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2a) |
|  | A - B/(C | $\Gamma / K)$ | (3) |  |  |  |  |
|  | - B/(T) | - C•log (T/K) | (4) |  |  |  |  |
| Linder 1931 |  | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| mercury manometer |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -4.7 | 13.3 | 22.7 | 133.3 | 96.233 | 6415 | 62.35 | 1333 |
| 5.5 | 33.3 | 48.8 | 666.6 | 100.814 | 7697 | 76.32 | 2666 |
| 12.2 | 64 | 63 | 1333 | 104.778 | 8991 | 85.21 | 4000 |
|  |  | 76.3 | 2666 | 108.403 | 10328 | 91.86 | 5333 |
|  |  | 92.4 | 5333 | 111.762 | 11722 | 97.241 | 6666 |
|  |  | 102.6 | 7999 | 116.322 | 13840 | 101.785 | 7999 |
|  |  | 116.2 | 13332 | 121.506 | 16640 | 109.243 | 10666 |
|  |  | 136.9 | 26664 | 126.797 | 19945 | 115.286 | 13332 |
|  |  | 159.2 | 53329 | 138.3 | 28979 | 126.89 | 19998 |
|  |  | 183.1 | 101325 | 151.541 | 43352 | 135.853 | 26664 |
|  |  |  |  | 159.032 | 53693 | 142.779 | 33331 |
|  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -82.1 | 167.011 | 66793 | 149.829 | 39997 |
|  |  |  |  | 175.666 | 83753 | 158.82 | 53329 |
|  |  |  |  | 181.767 | 97645 | 166.971 | 66661 |
|  |  |  |  | 182.429 | 99245 | 173.91 | 79993 |
|  |  |  |  | 183.636 | 100734 | 179.985 | 93326 |
|  |  |  |  | 183.725 | 102456 | 181.116 | 95992 |
|  |  |  |  | 184.329 | 103989 | 182.223 | 98659 |
|  |  |  |  |  |  | 183.306 | 101325 |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  |  |  | A | 6.98318 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  | B | 1577.965 | A | 6.9808 |
|  |  |  |  | C | 201.378 | B | 1577.008 |
|  |  |  |  |  |  | C | 201.331 |
|  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 183.27 |  |  |
|  |  |  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 183.306 |
|  |  |  |  |  |  |  | ( $\mathrm{kJ} \mathrm{mol}^{-1}$ ) |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 50.12 |
|  |  |  |  |  |  | at bp | 37.75 |



FIGURE 3.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-butylbenzene.

### 3.1.1.17 Isobutylbenzene



Common Name: Isobutylbenzene
Synonym: i-butylbenzene, 2-methylpropylbenzene, methyl-1-phenylpropane
Chemical Name: isobutylbenzene
CAS Registry No: 538-93-2
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}_{2} \mathrm{CH}\left(\mathrm{CH}_{3}\right)_{2}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -51.4 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 170.5 (Stephenson \& Malanowski 1987)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8532 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$157.3 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 12.51 (Dreisbach 1955)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ : 10.1 (shake flask-GC, Price 1976)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
667* (21.1 ${ }^{\circ} \mathrm{C}$, summary of literature data, Stull 1947)
6415* $\quad\left(86.637^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $86.637-173.814^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93033-1526.384 /\left(204.171+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $86.6-173.8^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
257 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.93033-1526.384 /\left(204.171+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-210^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
248* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92804-1525.446 /\left(204.122+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $53.21-202.45^{\circ} \mathrm{C}$ (liquid, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 8567.8 /(\mathrm{T} / \mathrm{K})]+7.048112$; temp range: -9.8 to $170.5^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{atm})=(1-445.940 / \mathrm{T}) \times 10^{\wedge}\left(0.870338-6.75481 \times 10^{4} \cdot \mathrm{~T}+5.59009 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 285.0-645.0 K (Cox vapor pressure eq., Chao et al. 1983)

249 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.06156-1530.811 /\left(204.675+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $86.64-173.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.06898-1536.514 /(-67.788+\mathrm{T} / \mathrm{K})$; temp range $373-447 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-7.0438-2.6892 \times 10^{3} /(\mathrm{T} / \mathrm{K})+8.7843 \cdot \log (\mathrm{~T} / \mathrm{K})-2.1426 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+1.1248 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 222-650 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
1160, 1714 (calculated- $\mathrm{C}_{\mathrm{W}} / \mathrm{C}_{\mathrm{A}}$, calculated-bond contribution, Hine \& Mookerjee 1975)
3300 (calculated-P/C, Mackay \& Shiu 1981)
1393 (calculated-QSAR, Nirmalakhandan \& Speece 1988b)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.01 (headspace GC, Hutchinson et al. 1980)
4.54, 4.82 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.68 (average lit. value, Sangster 1993)
4.54 (Hansch et al. 1995)

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants or Half-Lives:
Volatilization: estimated $t_{1 / 2} \sim 3.2 \mathrm{~h}$, evaporation from a river of 1 m depth with wind speed $3 \mathrm{~m} / \mathrm{s}$ and water current of $1 \mathrm{~m} / \mathrm{s}$ at $20^{\circ} \mathrm{C}$ (Lyman et al. 1982).

Half-Lives in the Environment:

TABLE 3.1.1.17.1
Reported vapor pressures of isobutylbenzene at various temperatures and the coefficients for vapor pressure equations

|  | 1947 | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summa | terature data | ebulliometry |  | selected values |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |  |
| -9.8 | 133.3 | 86.637 | 6415 | 53.21 | 1333 |  |
| 21.1 | 666.6 | 91.118 | 7697 | 66.97 | 2666 |  |
| 37.3 | 1333 | 95.026 | 8991 | 75.73 | 4000 |  |
| 54.7 | 2666 | 98.62 | 10328 | 82.29 | 5333 |  |
| 73.2 | 5333 | 101.946 | 11722 | 87.602 | 6666 |  |
| 84.1 | 7999 | 106.45 | 13840 | 92.087 | 7999 |  |
| 99 | 13332 | 111.582 | 16640 | 99.452 | 10666 |  |
| 120.7 | 26664 | 116.808 | 19945 | 105.422 | 13332 |  |
| 145.2 | 53329 | 121.659 | 23474 | 116.893 | 19998 |  |
| 170.2 | 101325 | 128.149 | 28979 | 125.561 | 26664 |  |
|  |  | 134.112 | 34918 | 132.614 | 33331 |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | 141.301 | 43352 | 138.694 | 39997 |  |
|  |  | 148.724 | 53693 | 149.502 | 53329 |  |
|  |  | 156.632 | 66793 | 156.583 | 66661 |  |
|  |  | 165.217 | 83754 | 163.465 | 79993 |  |
|  |  | 171.27 | 97647 | 169.492 | 93326 |  |
|  |  | 171.92 | 99247 | 170.615 | 95992 |  |
|  |  | 172.526 | 100737 | 171.714 | 98659 |  |
|  |  | 173.209 | 102457 | 172.789 | 101325 |  |
|  |  | 173.814 | 103990 |  |  |  |
|  |  |  |  | $\text { eq. } 2$ | $\mathrm{P} / \mathrm{mmHg}$ |  |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | A | $6.92804$ |  |
|  |  | A | $6.93033$ | B | 1525.446 |  |
|  |  | B | $1526.384$ | C | 204.122 |  |
|  |  | C | 204.171 | bp/ ${ }^{\circ} \mathrm{C}$ | 172.789 |  |
|  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |
|  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 172.759 | at $25^{\circ} \mathrm{C}$ | 49.45 |  |
|  |  |  |  | at bp | 37.82 |  |



FIGURE 3.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for isobutylbenzene.

### 3.1.1.18 sec-Butylbenzene



Common Name: sec-Butylbenzene
Synonym: 2-phenylbutane, (1-methylpropyl)benzene, $s$-butylbenzene
Chemical Name: sec-butylbenzene
CAS Registry No: 135-98-8
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}\left(\mathrm{CH}_{3}\right) \mathrm{C}_{2} \mathrm{H}_{5}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -82.7 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 173.3 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8621 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $155.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density) 184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 9.83 (Dreisbach 1955)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
30.9 (shake flask-UV, Andrews \& Keefer 1950)
17.6 (shake flask-GC, Sutton \& Calder 1975)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$70.7^{*} \quad\left(9.8^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -8.6 to $9.8^{\circ} \mathrm{C}$, Linder 1931)
133.3* ( $18.6^{\circ} \mathrm{C}$, summary of literature data, temp range $18.6-173.5^{\circ} \mathrm{C}$, Stull 1947)
$6415^{*} \quad\left(87.118^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $87.118-174.358^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\left.\log (\mathrm{P} / \mathrm{mmHg})=6.95097-1540.174 /(205.101+\mathrm{t})^{\circ} \mathrm{C}\right)$; temp range $87.1-174.4^{\circ} \mathrm{C}$, (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
250 (extrapolated, Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95097-1540.174 /\left(205.101+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-210^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
241* (extrapolated, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.94866-1539.233 /\left(205.052+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $53.7-202.95^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 11609.3 /(\mathrm{T} / \mathrm{K})]+8.318014 ;$ temp range $18.6-173.5^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-446.499 / \mathrm{T}) \times 10^{\wedge}\left(0.870844-6.72060 \times 10^{4} \cdot \mathrm{~T}+5.52698 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 285.0-645.0 K (Cox vapor pressure eq., Chao et al. 1983)

240 (extrapolated, Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.05072-1533.897 /\left(204.382+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $87.12-174.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=6.94219-1533.95 /\left(204.39+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $87-174^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.10298-1559.452 /(\mathrm{C}+\mathrm{T} / \mathrm{K})$; temp range $384-448 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

188* (20.33 ${ }^{\circ} \mathrm{C}$, static method, measured range 243.92-373.39 K, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{kPa})=6.47915-1781.723 /\left(208.35+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $243.92-373.39 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=61.5904-4.5093 \times 10^{3} /(\mathrm{T} / \mathrm{K})-19.522 \cdot \log (\mathrm{~T} / \mathrm{K})+6.9865 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+7.8205 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 198-665 K (Yaws 1994)
$186^{*} \quad\left(20.23^{\circ} \mathrm{C}\right.$, static method, measured range 263.52-393.39 K, Mokbel et al. 1998)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.44, 4.70 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.57 (average lit. value, Sangster 1993)
4.44 (Hansch et al. 1995)
3.90 (computed-expert system SPARC, Kollig 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
2.71 (aquifer material with $\mathrm{f}_{\mathrm{OC}}$ of 0.006 and measured partition coeff. $\mathrm{K}_{\mathrm{P}}=3.06 \mathrm{~mL} / \mathrm{g}$., Abdul et al. 1990)
3.60 (computed- $\mathrm{K}_{\mathrm{OW}}$, Kollig 1995)

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

TABLE 3.1.1.18.1
Reported vapor pressures of sec-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |  |

1. 

| Linder 1931 |  | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -8.6 | 13.33 | 18.6 | 133.3 | 87.118 | 6415 | 53.7 | 1333 |
| -3.0 | 24 | 44.2 | 666.6 | 91.684 | 7695 | 67.49 | 2666 |
| 2.6 | 42.66 | 57 | 1333 | 95.62 | 8990 | 76.26 | 4000 |
| 9.8 | 70.66 | 70.6 | 2666 | 99.179 | 10328 | 82.84 | 5333 |
|  |  | 86.2 | 5333 | 102.523 | 11722 | 88.15 | 6666 |
|  |  | 96 | 7999 | 107.009 | 13840 | 92.614 | 7999 |
|  |  | 109.5 | 13332 | 112.151 | 16641 | 100.012 | 10666 |
|  |  | 128.8 | 26664 | 117.387 | 19945 | 105.986 | 13332 |
|  |  | 150.3 | $53329$ | 122.232 | 23475 | 117.462 | 19998 |
|  |  | 173.5 | 101325 | 128.715 | 28979 | 126.132 | 26664 |
|  |  |  |  | 134.683 | 43352 | 133.185 | 33331 |
|  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -82.87 | 141.867 | 53693 | 139.175 | 39997 |
|  |  |  |  | 149.288 | 66793 | 149.069 | 53329 |
|  |  |  |  | $157.194$ | 83754 | 157.133 | 66661 |
|  |  |  |  | 165.768 | 97647 | 164.021 | 79993 |

TABLE 3.1.1.18.1 (Continued)
1.

| Linder 1931 |  | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| mercury manometer |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  |  |  | 171.82 | 99245 | 170.042 | 93326 |
|  |  |  |  | 173.068 | 100737 | 171.164 | 95992 |
|  |  |  |  | 173.754 | 102457 | 172.261 | 98659 |
|  |  |  |  | 174.358 | 103990 | 173.864 | 101325 |
|  |  |  |  | $\text { eq. } 2$ | $\mathrm{P} / \mathrm{mmHg}$ | $\text { eq. } 2$ | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  | A | $6.95097$ | A | 6.94866 |
|  |  |  |  | B | 1540.174 | B | 1539.223 |
|  |  |  |  | C | 205.101 | C | 205.052 |
|  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 173.035 | bp/ ${ }^{\circ} \mathrm{C}$ | 173.335 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=$ |  |
|  |  |  |  |  |  | $\text { at } 25^{\circ} \mathrm{C}$ | $49.5$ |
|  |  |  |  |  |  | at bp | $37.95$ |

2. 

| Kasehgari et al. 1993 |  | Mokbel et al. 1998 |  |
| :---: | :---: | :---: | :---: |
| static method |  | static method |  |
| T/K | $\mathbf{P / P a}$ | T/K | P/Pa |
| 243.92 | 2.92 | 263.52 | 16.31 |
| 253.79 | 7.99 | 273.42 | 43.34 |
| 263.69 | 19.3 | 283.40 | 92.39 |
| 273.55 | 44.9 | 293.38 | 186.0 |
| 283.50 | 93.3 | 303.42 | 357.0 |
| 293.48 | 188 | 313.44 | 652.0 |
| 303.49 | 358 | 323.55 | 1145 |
| 313.61 | 654 | 333.55 | 1943 |
| 313.61 | 655 | 343.57 | 3088 |
| 323.60 | 1136 | 353.62 | 4862 |
| 323.60 | 1139 | 363.43 | 7329 |
| 328.60 | 1478 | 373.39 | 10789 |
| 333.57 | 1904 |  |  |
| 343.57 | 3088 | data fitte | Wagner eq. |
| 363.43 | 4862 |  |  |
| 373.39 | 7329 |  |  |
|  | Antoine eq. |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{kPa}$ |  |  |
| A | 6.479 |  |  |
| B | 1781.723 |  |  |
| C | 226.989 |  |  |



FIGURE 3.1.1.18.1 Logarithm of vapor pressure versus reciprocal temperature for sec-butylbenzene.

### 3.1.1.19 tert-Butylbenzene



Common Name: tert-Butylbenzene
Synonym: (1,1-dimethylethyl)benzene, 2-methyl-2-phenylpropane, trimethylphenylmethane, pseudobutylbenzene, $t$ butylbenzene
Chemical Name: tert-butylbenzene
CAS Registry No: 98-06-6
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{C}\left(\mathrm{CH}_{3}\right)_{3}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-58 (Stephenson \& Malanowski 1987)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
169.1 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8665 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$154.9 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
8.38 (Dreisbach 1955)
8.40 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
39.1, 45.4 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
34.0 (shake flask-UV, Andrews \& Keefer 1950)
29.5 (shake flask-GC, Sutton \& Calder 1975)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$144^{*} \quad\left(13.7^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -2 to $13.7^{\circ} \mathrm{C}$, Linder 1931)
$133.3^{*} \quad\left(13^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $13-168.5^{\circ} \mathrm{C}$, Stull 1947)
$6426^{*} \quad\left(83.887^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $83.887-170.165^{\circ} \mathrm{C}$, Forziati et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=9.2050-1504.572 /\left(203.328+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $83.9-170.2^{\circ} \mathrm{C}$ (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
295 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92050-1504.572 /\left(203.328+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $70-205^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
286* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.91829-1503.651 /\left(203.280+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $50.79-198.54^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10705.5 /(\mathrm{T} / \mathrm{K})]+8.195269$; temp range $13-168^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{atm})=(1-442.319 / \mathrm{T}) \times 10^{\wedge}\left(0.881530-7.21114 \times 10^{4} \cdot \mathrm{~T}+6.01764 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 285.0-635.0 K (Cox vapor pressure eq., Chao et al. 1983)

285 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.03861-1499.886 /\left(202.792+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $83.88-170.2^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)
286 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92255-1505.987 /\left(203.49+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $84-170^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.06067-1515.51 /(-68.551+\mathrm{T} / \mathrm{K})$; temp range $368-444 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=41.4522-3.9027 \times 10^{3} /(\mathrm{T} / \mathrm{K})-11.410 \cdot \log (\mathrm{~T} / \mathrm{K})+2.4320 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+2.2517 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $215-660 \mathrm{~K}$ (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
1200 (calculated-P/C, Mackay \& Shiu 1981)
1300 (calculated $-\mathrm{C}_{\mathrm{A}} / \mathrm{C}_{\mathrm{W}}$, Eastcott et al. 1988)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.11 (Leo et al. 1971; Hansch \& Leo 1979)
4.07 (shake flask-HPLC, Nahum \& Horvath 1980)
4.25, 4.49 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.11 (recommended, Sangster 1989, 1993)
4.11 (recommended, Hansch et al. 1995)
3.73 (RP-HPLC-RT correlation, short ODP column, Donovan \& Pescatore 2002)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization/Evaporation:
Photolysis:
Oxidation: rate constant $\mathrm{k}=4.58 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the gas phase reaction with OH radical at room temp. (Ohta \& Ohyama 1985; Atkinson 1989);
rate constant $\mathrm{k}=4.6 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the gas-phase reaction with OH radical at 298 K (Atkinson 1990).

Oxidation:
Hydrolysis:
Biodegradation:
Bioconcentration
Half-Lives in the Environment:

TABLE 3.1.1.19.1
Reported vapor pressures of tert-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | (1) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B}$ | T/K) | (1a) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |  | (2) |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B}$ | C $\left.+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2a) |
| $\log P=A-B /(C+T / K)$ |  |  | (3) |  |  |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K}) \quad$ (4) |  |  |  |  |  |  |  |
| Linder 1931 |  | Stull 1947 |  | Forziati et al. 1949 |  | Zwolinski \& Wilhoit 1971 |  |
| mercury manometer |  | summary of literature data |  | ebulliometry |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -2.0 | 36 | 13 | 133.3 | 83.887 | 6426 | 50.79 | 1333 |
| 2.3 | 57.3 | 39 | 666.6 | 88.312 | 7695 | 64.41 | 2666 |
| 10.8 | 140 | 51.7 | 1333 | 92.194 | 8990 | 73.07 | 4000 |
| 13.7 | 144 | 65.6 | 2666 | 95.715 | 10332 | 79.56 | 5333 |
|  |  | 80.8 | 5333 | 99.017 | 11722 | 84.816 | 6666 |
|  |  | 90.6 | 7999 | 103.471 | 13840 | 89.254 | 7999 |
|  |  | 103.8 | 13332 | 108.546 | 16641 | 96.542 | 10666 |
|  |  | 123.7 | 26664 | 113.72 | 19945 | 102.449 | 13332 |
|  |  | 145.8 | 53329 | 118.524 | 23475 | 113.802 | 19998 |
|  |  | 168.5 | 101325 | 124.936 | 28979 | 122.449 | 26664 |
|  |  |  |  | 137.968 | 43354 | 129.364 | 33331 |
|  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -58.0 | 145.315 | 53692 | 135.295 | 39997 |
|  |  |  |  | 153.149 | 66781 | 145.095 | 53329 |
|  |  |  |  | 161.649 | 83754 | 153.097 | 66661 |
|  |  |  |  | 167.646 | 97647 | 159.913 | 79993 |
|  |  |  |  | 168.287 | 99247 | 165.882 | 93326 |
|  |  |  |  | 168.886 | 100737 | 166.994 | 95992 |
|  |  |  |  | 169.565 | 102458 | 168.083 | 98659 |
|  |  |  |  | 170.165 | 103991 | 169.018 | 101325 |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  | A | 6.9205 | A | 6.91829 |
|  |  |  |  | B | 1504.572 | B | 1503.651 |
|  |  |  |  | C | 203.328 | C | 203.28 |
|  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 169.119 | bp/ ${ }^{\circ} \mathrm{C}$ | 169.148 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{V}}$ | $\left.\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | 49.8 |
|  |  |  |  |  |  | at bp | 37.61 |



FIGURE 3.1.1.19.1 Logarithm of vapor pressure versus reciprocal temperature for tert-butylbenzene.

### 3.1.1.20 1,2,3,4-Tetramethylbenzene



Common Name: 1,2,3,4-Tetramethylbenzene
Synonym: perhintene, prebnitene
Chemical Name: 1,2,3,4-tetramethylbenzene
CAS Registry No: 488-23-3
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{2}\left(\mathrm{CH}_{3}\right)_{4}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-6.2 (Weast 1982-83; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
205 (Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.9052 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$148.3 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
11.21 (Dreisbach 1955)
11.23 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
42.31, 45.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$133.3^{*} \quad\left(42.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $42.6-204.4^{\circ} \mathrm{C}$, Stull 1947)
49.20 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0584-1689.10 /\left(199.28+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $100-250^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1333* $\quad\left(79.515^{\circ} \mathrm{C}\right.$, compiled data, temp range $79.515-235.815^{\circ} \mathrm{C}$, Bond \& Thodos 1960)
45.01* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0594-1690.54 /\left(199.48+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $79.5-235.9^{\circ} \mathrm{C}$ (liquid, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 12258.0 /(\mathrm{T} / \mathrm{K})]+8.534237$; temp range $42.6-204.4^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) $\log (\mathrm{P} / \mathrm{atm})=(1-478.255 / \mathrm{T}) \times 10^{\wedge}\left(0.889494-6.47585 \times 10^{4} \cdot \mathrm{~T}+4.96841 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 310.0-690.0 K (Cox vapor pressure eq., Chao et al. 1983)
45.01 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0594-1690.54 /\left(199.48+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $80-217^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
45.02 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1843-1690.54 /(-73.67+\mathrm{T} / \mathrm{K})$; temp range $352-509 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.84 (generator column-HPLC, Wasik et al. 1982)
4.11 (HPLC-k' correlation, Hammers et al. 1982)
4.30, 4.53 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.00 (recommended, Sangster 1989, 1993)
4.09 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
3.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.20.1
Reported vapor pressures of 1,2,3,4-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  |  | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\begin{aligned} & (1 a) \\ & (2 a) \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |  |  | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ |  |  |  | (3) |  |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ |  |  |  | (4) |  |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})+\mathrm{D} \cdot \mathrm{P} /(\mathrm{T} / \mathrm{K})^{2}$ |  |  |  | (5) |  |  |  |
|  | 1947 | Bond \& | dos 1960 | Zwolinski \& Wilhoit 1971 |  |  |  |
| summary of literature data |  | compiled data |  | selected values |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 42.6 | 133.3 | 79.515 | 1333 | 79.5 | 1333 | 201.6 | 93326 |
| 68.7 | 666.6 | 128.415 | 10666 | 94.1 | 2666 | 202.83 | 95992 |
| 81.8 | 1333 | 188.185 | 66661 | 103.4 | 4000 | 204.54 | 98659 |
| 95.8 | 2666 | 216.925 | 133322 | 110.3 | 5333 | 205.09 | 101325 |
| 111.5 | 5333 | 235.815 | 199984 | 115.9 | 6666 |  |  |
| 121.8 | 7999 |  |  | 120.6 | 7999 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 135.7 | 13332 | bp/ ${ }^{\circ} \mathrm{C}$ | 205.055 | 128.4 | 10666 | A | 7.0594 |
| 1155.7 | 26664 |  |  | 134.7 | 13332 | B | 1690.54 |
| 180 | 53329 | eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ | 146.7 | 19998 | C | 199.48 |
| 204.4 | 101325 | A | 27.4323 | 155.8 | 26664 | bp/ ${ }^{\circ} \mathrm{C}$ | 205.9 |
|  |  | B | 3713.52 | 163.2 | 33331 | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -4.0 | C | 6.77416 | 169.2 | 39997 | at $25^{\circ} \mathrm{C}$ | 57.15 |
|  |  | D | 3.81118 | 179.8 | 53329 | at bp | 45.02 |
|  |  |  |  | 188.22 | 66661 |  |  |
|  |  |  |  | 195.99 | 79993 |  |  |



FIGURE 3.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,4-tetramethylbenzene.

### 3.1.1.21 1,2,3,5-Tetramethylbenzene



Common Name: 1,2,3,5-Tetramethylbenzene
Synonym: isodurene
Chemical Name: 1,2,3,5-tetramethylbenzene
CAS Registry No: 527-53-7
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{2}\left(\mathrm{CH}_{3}\right)_{4}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-24.1 (Stephenson \& Malanowski 1987)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
198 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8903 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$150.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 12.93 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 52.01, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
16.2, 16.4, $19.4 \quad\left(15,25,35^{\circ} \mathrm{C}\right.$, estimated- RP-HPLC-k' correlation, Finizio \& Di Guardo 2001)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* ( $40.6^{\circ} \mathrm{C}$, summary of literature data, temp range $40.6-197.9^{\circ} \mathrm{C}$, Stull 1947)
67.10 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0769-1674.00 /\left(200.94+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $95-240^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
62.22* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.70779-1675.43 /\left(201.14+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $74.5-228.3^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 12358.4 /(\mathrm{T} / \mathrm{K})]+8.680246$; temp range $40.6-197.9^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73) $\log (\mathrm{P} / \mathrm{atm})=(1-471.208 / \mathrm{T}) \times 10^{\wedge}\left(0.891876-6.64575 \times 10^{4} \cdot \mathrm{~T}+5.21861 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 305.0-675.0 K (Cox vapor pressure eq., Chao et al. 1983)
62.22 (extrapolated, Antoine eq., Dean 1985)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0779-1675.43 /\left(201.14+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-228^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
62.23 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.2028-1675.43 /(-72.01+\mathrm{T} / \mathrm{K})$; temp range $348-502 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-3.9778-2.960 \times 10^{3} /(\mathrm{T} / \mathrm{K})+7.3226 \cdot \log (\mathrm{~T} / \mathrm{K})-1.7725 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+8.6365 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 249-679 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.04 (generator column-HPLC/UV, Wasik et al. 1982)
4.17 (HPLC-k' correlation, Hammers et al. 1982)
4.30 (average value, RP-HPLC-k' correlation, Sherblom \& Eganhouse 1988)
4.10 (recommended, Sangster 1989, 1993)
4.23 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
4.04 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.21.1
Reported vapor pressures of 1,2,3,5-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log P=A-B /(T / K)$ |  | $\ln P=A-B /(T / K)$ |
| ---: | :--- | ---: | :--- |
| $\log P=A-B /\left(C+t /{ }^{\circ} C\right)$ | $(2)$ | $\ln P=A-B /\left(C+t /{ }^{\circ} C\right)$ |
| $\log P=A-B /(C+T / K)$ | (3) |  |
| $\log P=A-B /(T / K)-C \cdot \log (T / K)$ | (4) |  |

Stull 1947
Zwolinski \& Wilhoit 1971

| summary of literature data |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 40.6 | 133.3 | 74.5 | 1333 | 194.68 | 93326 |
| 65.8 | 666.6 | 88.9 | 2666 | 195.83 | 95992 |
| 77.8 | 1333 | 98 | 4000 | 196.95 | 98659 |
| 91 | 2666 | 104.8 | 5333 | 198.05 | 101325 |
| 105.8 | 5333 | 110.3 | 6666 |  |  |
| 115.4 | 7999 | 115 | 7999 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 128.3 | 13332 | 122.6 | 10666 | A | 7.0779 |
| 149.9 | 26664 | 128.8 | 13332 | B | 1675.43 |
| 173.7 | 53329 | 140.7 | 19998 | C | 201.14 |
| 197.9 | 101325 | 149.6 | 26664 |  |  |
|  |  | 156.9 | 33331 | bp/ ${ }^{\circ} \mathrm{C}$ | 198.05 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -24.0 | 163 | 39997 | $\Delta \mathrm{H}_{\mathrm{v}} /$ | $\left.\mathrm{mol}^{-1}\right)=$ |
|  |  | 173.2 | 53329 | at $25^{\circ} \mathrm{C}$ | 55.82 |
|  |  | 181.5 | 66661 | at bp | 43.81 |
|  |  | 188.5 | 79993 |  |  |



FIGURE 3.1.1.21.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetramethylbenzene.

### 3.1.1.2 1,2,4,5-Tetramethylbenzene



Common Name: 1,2,4,5-Tetramethylbenzene
Synonym: durene
Chemical Name: 1,2,4,5-tetramethylbenzene
CAS Registry No: 95-93-2
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{14}, \mathrm{C}_{6} \mathrm{H}_{2}\left(\mathrm{CH}_{3}\right)_{4}$
Molecular Weight: 134.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
79.3 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
196.8 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.838
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$160.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
21.0 (Dreisbach 1955; Tsonopoulos \& Prausnitz 1971)
20.88 (Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
59.83 (Tsonopoulos \& Prausnitz 1971)
59.25, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.293 ( mp at $79.3^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
19.5 (Deno \& Berkheimer 1960)
3.48 (shake flask-GC, Price 1976)
3.48 (shake flask-GC, Krzyzanowska \& Szeliga 1978)
13.9 (HPLC-k' correlation, converted from reported activity coeff $\gamma_{\mathrm{w}}$, Hafkenscheid \& Tomlinson 1983)
17.2, 18.6, $28.2 \quad\left(15,25,35^{\circ} \mathrm{C}\right.$, RP-HPLC-k' correlation, Finizio \& Di Guardo 2001)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$4.4^{*} \quad\left(1.75^{\circ} \mathrm{C}\right.$, mercury manometer, measured range $-1.7-1.75^{\circ} \mathrm{C}$, Linder 1931)
$133.3^{*} \quad\left(45^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $45-195.9^{\circ} \mathrm{C}$, Stull 1947)
70.9 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0790-1671.0 /\left(201.23+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $95-240^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
65.9* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0800-1672.43 /\left(201.43+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $73.6-227^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 12582.6 /(\mathrm{T} / \mathrm{K})]+8.822113$; temp range $45-195.9^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) $\log (\mathrm{P} / \mathrm{atm})=(1-470.032 / \mathrm{T}) \times 10^{\wedge}\left(0.884259-6.36677 \times 10^{4} \cdot \mathrm{~T}+4.97646 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 346.75-675.0 K (Cox vapor pressure eq., Chao et al. 1983)
65.9 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0800-1672.43 /\left(201.43+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $74-277^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
65.9 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.2049-1672.43 /(-71.72+\mathrm{T} / \mathrm{K})$; temp range 353-500 K (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-51.3593-1.6523 \times 10^{3} /(\mathrm{T} / \mathrm{K})+26.656 \cdot \log (\mathrm{~T} / \mathrm{K})-3.5721 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.5018 \times 10^{-5} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 352-Y675K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
2541 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
$4.00 \quad$ (Hansch \& Leo 1979)
4.24 (HPLC-RV correlation, Garst 1984)
4.13, 4.34 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.10 (recommended, Sangster 1989, 1993)
4.27 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
4.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.12 (average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach \& Westall 1981)
2.99 (soil, calculated-MCI $\chi$, Sabljic 1987a,b)
2.76 (aquifer material with $\mathrm{f}_{\mathrm{OC}}$ of 0.006 and measured $\mathrm{K}_{\mathrm{P}}=3.42 \mathrm{~mL} / \mathrm{g}$., Abdul et al. 1990)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $\mathrm{k}=1.1 \times 10^{4} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for reaction with ozone at 300 K (estimated, Lyman 1982).
Hydrolysis:
Biodegradation:
Bioconcentration:
Half-Lives in the Environment:

TABLE 3.1.1.22.1
Reported vapor pressures of 1,2,4,5-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations



FIGURE 3.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2,4,5-tetramethylbenzene.

### 3.1.1.23 Pentamethylbenzene



Common Name: Pentamethylbenzene
Synonym:
Chemical Name: pentamethylbenzene
CAS Registry No: 700-12-9
Molecular Formula: $\mathrm{C}_{11} \mathrm{H}_{16}, \mathrm{C}_{6} \mathrm{H}\left(\mathrm{CH}_{3}\right)_{5}$
Molecular Weight: 148.245
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
54.5 (Weast 1982-83; Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
232 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 0.917, $0.913 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
0.917 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$161.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
207.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$12.34 \quad$ (Tsonopoulos \& Prausnitz 1971)
$1.98,10.67 ; 12.65 \quad\left(23.65,55.05^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
$37.70 \quad$ (Tsonopoulos \& Prausnitz 1971)
39.33, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} . \mathrm{mol} \mathrm{K}$.), F: $0.514\left(\mathrm{mp}\right.$ at $54.5^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
15.6 (Deno \& Berkheimer 1960)
15.52 (calculated- $\mathrm{K}_{\text {Ow }}$, Yalkowsky et al. 1983)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
13.84 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.13756-1833.8 /\left(199.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $125-280^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
9.52 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.3509-1867 /(-75.15+\mathrm{T} / \mathrm{K})$; temp range $338-503 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
4.56 (HPLC-k' correlation, Hammers et al. 1982)
4.57 (HPLC-RV correlation, Garst 1984)
4.56 (recommended, Sangster 1989, 1993)
4.59 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
4.56 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 3.1.1.24 Pentylbenzene



Common Name: $n$-Pentylbenzene
Synonym: phenylpentane
Chemical Name: pentylbenzene
CAS Registry No: 538-68-1
Molecular Formula: $\mathrm{C}_{11} \mathrm{H}_{16}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{4} \mathrm{CH}_{3}$
Molecular Weight: 148.245
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-75 (Dreisbach 1955; Weast 1982-83; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
205.4 (Weast 1982-83; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8585 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$172.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
207.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
10.5 (shake flask-UV, Andrews \& Keefer 1950)
3.84 (generator column-HPLC/UV, Tewari et al. 1982c)
3.37* (generator column-HPLC/UV, measured range $7-45^{\circ} \mathrm{C}$, Owens et al. 1986)
$\ln x=-387.920+16274.64 /(\mathrm{T} / \mathrm{K})+55.9266 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
43.7 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.04709-1670.68 /\left(195.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $105-270^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
43.7* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.97833-1639.91 /\left(194.76+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $80-237^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=34.2755-3.6829 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.3387 \cdot \log (\mathrm{~T} / \mathrm{K})+2.7727 \times 10^{-3} .(\mathrm{T} / \mathrm{K})-8.8315 \times 10^{-15} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 198-680 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

| 600 | (calculated-P/C, Mackay \& Shiu 1981) |
| :--- | :--- |
| 617 | (calculated-C $/$ C $_{\mathrm{W}}$, Eastcott et al. 1988) |
| 1689 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |
| 1628.2 | (modified EPICS method-GC, Ryu \& Park 1999) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.56 (HPLC-k' correlation, Hammers et al. 1982)
4.90 (generator column-HPLC/UV, Tewari et al. 1982c)
4.90 (recommended, Sangster 1989, 1993)
4.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environment Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $\mathrm{k}=5.0 \times 10^{4} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone at 300 K (Lyman 1982).
Hydrolysis:
Biodegradation:
Bioconcentration:
Half-Lives in the Environment:

TABLE 3.1.1.24.1
Reported aqueous solubilities and vapor pressures of $n$-pentylbenzene at various temperatures

| Aqueous solubility | Vapor pressure |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| Owens et al. 1986 | Zwolinski \& Wilhoit 1971 |  |  |  |
| generator column-HPLC | selected values |  |  |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 73.48 | 80 | 1333 | 283.18 | 95992 |
| $10 \quad 3.18$ | 94 | 2666 | 203.16 | 97325 |
| 12.5 3.44 | 103.3 | 4000 | 204.33 | 98659 |
| 15 3.19 | 110.3 | 5333 | 204.9 | 99992 |
|  | 115.87 | 6666 | 205.46 | 101325 |
| 20 3.18 | 120.6 | 7999 |  |  |
| $25 \quad 3.37$ | 128.36 | 10666 | $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| $30 \quad 3.61$ | 134.65 | 13332 | Antoine eq. | $\mathrm{P} / \mathrm{mmHg}$ |
| $35 \quad 3.92$ | 146.73 | 19998 | A | 6.97833 |
| $40 \quad 4.25$ | 155.85 | 26664 | B | 1639.91 |
| $45 \quad 4.69$ | 163.27 | 33331 | C | 194.76 |
|  | 169.57 | 39997 |  |  |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=6.50$at $25^{\circ} \mathrm{C}$ | 179.97 | 53329 | bp/ ${ }^{\circ} \mathrm{C}$ | 205.46 |
|  | 188.45 | 66661 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ} \mathrm{mo}$ |  |
|  | 196.68 | 79993 | at $25^{\circ} \mathrm{C}$ | 55.06 |
|  | 202 | 93326 | at $25^{\circ} \mathrm{C}$ | 41.21 |
|  | 202.59 | 94659 |  |  |



FIGURE 3.1.1.24.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for n -pentylbenzene.


FIGURE 3.1.1.24.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-pentylbenzene.

### 3.1.1.25 Hexamethylbenzene



Common Name: $n$-Hexamethylbenzene
Synonym: mellitene
Chemical Name: $n$-hexamethylbenzene
CAS Registry No: 87-95-4
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{18}, \mathrm{C}_{6}\left(\mathrm{CH}_{3}\right)_{6}$
Molecular Weight: 162.271
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
165.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 263.4 (Weast 1982-83)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $25^{\circ} \mathrm{C}$ ): 1.063 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$152.6 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
229.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 20.46 (Tsonopoulos \& Prausnitz 1971) 1.76, 20.63; $22.38 \quad\left(110.5,165.55^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : $46.44 \quad$ (Tsonopoulos \& Prausnitz 1971) 51.6, 47.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.042\left(\mathrm{mp}=166.5^{\circ} \mathrm{C}\right.$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.235 (generator column-GC, Doucette \& Andren 1988)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
1.004* $\quad\left(41.07^{\circ} \mathrm{C}\right.$, transpiration method, measured range $41-90.5^{\circ} \mathrm{C}$, Overberger et al. 1969)
$0.28^{*} \quad\left(30^{\circ} \mathrm{C}\right.$, diaphragm pressure gauge, measured range $30-70^{\circ} \mathrm{C}$, Ambrose et al. 1976)
0.160 (calculated-vapor pressure eq., Ambrose et al. 1976)
$\log (\mathrm{P} / \mathrm{Pa})=13.134-3855 /[(\mathrm{T} / \mathrm{K})-21]$; temp range $202-343 \mathrm{~K}$ (diaphragm pressure gauge measurements, Antoine eq., Ambrose et al. 1976)
$\log (\mathrm{P} / \mathrm{atm})=(1-571.163 / \mathrm{T}) \times 10^{\wedge}\left(1.00973-5.04725 \times 10^{4} \cdot \mathrm{~T}-6.310130 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 303.1-343.02 K (Cox vapor pressure eq., Chao et al. 1983)
0.155 (extrapolated, Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=8.6223-2965.633 /(-59.583+\mathrm{T} / \mathrm{K})$; temp range $303-343 \mathrm{~K}$ (solid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.89588-1629.9 /(-118.46+\mathrm{T} / \mathrm{K})$; temp range $443-537 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson $\&$ Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.61 (generator column-HPLC, Wasik et al. 1982)
5.11 (HPLC-k' correlation, Hammers et al. 1982)
4.31 (HPLC-RV correlation, Garst \& Wilson 1984)
4.60 (shake flask/slow stirring-GC, Brooke et al. 1986)
4.60, 4.88 (reversed phase HPLC-k' correlations, Sherblom \& Eganhouse 1988)
4.75 (recommended, Sangster 1989)
4.95 (normal phase HPLC-k' correlation, Govers \& Evers 1992)
5.11 (recommended, Sangster 1993)
4.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
6.31 (calculated- $\mathrm{S}_{\text {oct }}$ and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $\mathrm{k}=2.4 \times 10^{5} \mathrm{~cm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone at 300 K (Lyman et al. 1982)
Hydrolysis:
Biodegradation:
Bioconcentration
Half-Lives in the Environment:

TABLE 3.1.1.25.1
Reported vapor pressures of hexamethylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |


| Overberger et al. 1969 |  | Ambrose et al. 1976 |  |
| :---: | :---: | :---: | :---: |
| transpiration method |  | diaphragm gauge |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 41.07 | 1.004 | 29.95 | 0.28 |
| 49.11 | 2.306 | 35.07 | 0.49 |
| 54.68 | 3.912 | 40.02 | 0.85 |
| 62.62 | 8.015 | 44.96 | 1.41 |
| 68.71 | 13.62 | 49.95 | 2.34 |
| 68.72 | 13.58 | 55.04 | 3.81 |
| 75.21 | 23.71 | 59.95 | 6.05 |
| 75.33 | 23.79 | 64.91 | 9.39 |
| 79.75 | 33.69 | 69.87 | 14.4 |
| 79.75 | 33.5 |  |  |
| 84.2 | 48.3 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 165.55 |
| 89.46 | 72 |  |  |
| 89.48 | 72.16 | eq. 3 | $\mathrm{P} / \mathrm{Pa}$ |
| 90.54 | 77.91 | A | 13.134 |
|  |  | B | 3855 |
|  |  | C | -21.0 |



FIGURE 3.1.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-hexamethylbenzene.

### 3.1.1.26 $n$-Hexylbenzene



Common Name: $n$-Hexylbenzene
Synonym: 1-phenylhexane, hexylbenzene
Chemical Name: $n$-hexylbenzene
CAS Registry No: 1077-16-3
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{18}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{5} \mathrm{CH}_{3}$
Molecular Weight: 162.271
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-61.0 (Dreisbach 1955; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
226.1 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.8613 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$188.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
229.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ}$ C, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.02 (generator column-HPLC/UV, Tewari et al. 1982c)
0.995* (generator column-HPLC, measured range $5-29^{\circ} \mathrm{C}$, May et al. 1983)
0.902* (generator column-HPLC/UV, measured range $7-45^{\circ} \mathrm{C}$, Owens et al. 1986)
$\ln x=-429.463+18024.83 /(\mathrm{T} / \mathrm{K})+61.9402 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $290-400 \mathrm{~K}$ (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
14.01 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.18284-1813.74 /\left(195.5+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $120-290^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
13.61* (extrapolated, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9853-1700.5 /\left(188.2+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $96-258^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971) $10.52^{*} \quad\left(20.51^{\circ} \mathrm{C}\right.$, static method, measured range 273.73-462.97 K, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{kPa})=6.50020-1946.435 /\left(208.935+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $273.73-462.97 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=6.7694-3.6050 \times 10^{3} /(\mathrm{T} / \mathrm{K})+3.3416 \cdot \log (\mathrm{~T} / \mathrm{K})-1.5306 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+7.8479 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $212-698 \mathrm{~K}$ (Yaws 1994)
10.52* ( $20.51^{\circ} \mathrm{C}$, measured range $263.88-462.97 \mathrm{~K}$, Mokbel et al. 1998)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
1977 (calculated-C ${ }_{A} / C_{\mathrm{W}}$, Eastcott et al. 1988)
2172 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
5.25 (calculated-fragment const., Rekker 1977)
5.52 (generator column-HPLC/UV, Tewari et al. 1982c)
5.24 (TLC-RT correlation, Bruggeman et al. 1982)
5.45, 5.25 (quoted of HPLC methods, Harnisch et al. 1983)
5.26, 5.62 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
5.52 (recommended, Sangster 1989, 1993)
5.52 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $t_{1 / 2}$ :

Half-Lives in the Environment:

TABLE 3.1.1.26.1
Reported aqueous solubilities of $n$-hexylbenzene at various temperatures
May et al. 1983

| generator column-HPLC |  |  |  | generator column-HPLC |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 5 | 0.921 | 20 | 0.043 | 7 | 0.834 |
| 6 | 0.921 | 21 | 0.949 | 10 | 0.836 |
| 8 | 0.92 | 22 | 0.956 | 15 | 0.826 |
| 9 | 0.996 | 23 | 0.953 | 20 | 0.951 |
| 11 | 0.904 | 24 | 0.983 | 25 | 0.902 |
| 12 | 0.928 | 25 | 0.995 | 30 | 0.996 |
| 13 | 0.93 | 26 | 0.999 | 35 | 1.069 |
| 14 | 0.92 | 27 | 0.999 | 40 | 1.069 |
| 15 | 0.925 | 29 | 1.012 | 45 | 1.298 |
| 16.01 | 0.908 | 29 | 1.016 |  |  |
| 17 | 0.919 | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=7.60$ |  | $\Delta \mathrm{H}_{\text {sol }}\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=8.0$ |  |
| 18 | 0.91 |  |  |  | at $25^{\circ} \mathrm{C}$ |
| 19 | 0.921 |  | at $25^{\circ} \mathrm{C}$ |  |  |



FIGURE 3.1.1.26.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $n$-hexylbenzene.

TABLE 3.1.1.26.2
Reported vapor pressures of $n$-hexylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | ---: | :--- | ---: |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |


| Zwolinski \& Wilhoit 1971 |  | Kasehgari et al. 1993 |  | Mokbel et al. 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| selected values |  | static method |  | static method |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathbf{P / P a}$ | T/K | P/Pa |
| 96 | 1333 | 273.73 | 1.653 | 263.88 | 0.609 |
| 111 | 2666 | 283.63 | 4.239 | 273.73 | 1.648 |
| 121 | 4000 | 293.66 | 10.52 | 283.63 | 4.236 |
| 128 | 5333 | 303.64 | 23.20 | 293.66 | 10.52 |
| 133.5 | 6666 | 313.62 | 48.66 | 303.64 | 23.20 |
| 138.4 | 7999 | 323.59 | 97.32 | 313.62 | 48.72 |
| 146.4 | 10666 | 333.58 | 184.9 | 323.59 | 97.36 |
| 152.9 | 13332 | 343.57 | 336.63 | 333.58 | 185.0 |
| 165.4 | 19998 | 353.58 | 589.1 | 343.57 | 336.0 |
| 174.8 | 26664 | 363.58 | 997.8 | 353.58 | 589.0 |
| 182.5 | 33331 | 372.84 | 1606 | 363.58 | 998.0 |
| 189.0 | 39997 | 382.77 | 2519 | 372.84 | 1606 |
| 199.8 | 53329 | 392.70 | 3841 | 382.77 | 2520 |
| 208.5 | 66661 | 402.74 | 5722 | 392.70 | 3841 |
| 216.0 | 79993 | 412.76 | 8320 | 402.74 | 5722 |
| 222.5 | 93326 | 422.76 | 11828 | 412.76 | 8321 |
| 223.1 | 94659 | 432.75 | 16516 | 422.76 | 11829 |
| 223.7 | 95992 | 442.89 | 22640 | 432.75 | 16517 |
| 224.3 | 97325 | 452.83 | 30575 | 442.80 | 22641 |
| 224.9 | 98659 | 462.97 | 40693 | 452.83 | 30576 |
| 225.5 | 99992 |  |  | 462.79 | 40694 |
| 226.1 | 101325 | eq. 2 | $\mathrm{P} / \mathrm{kPa}$ |  |  |
|  |  | A | 6.50020 | data fitted to Wagner eq. |  |
| Antoine eq. | $\mathrm{P} / \mathrm{mmHg}$ | B | 1946.435 |  |  |
| A | 6.9853 | C | 208.935 |  |  |
| B | 1700.5 |  |  |  |  |
| C | 1882.2 |  |  |  |  |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 226.1 |  |  |  |  |
| $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |  |  |  |  |
| at $25^{\circ} \mathrm{C}$ | 60 |  |  |  |  |
| at bp | 43.1 |  |  |  |  |



FIGURE 3.1.1.26.2 Logarithm of vapor pressure versus reciprocal temperature for $n$-hexylbenzene.

### 3.1.1.27 Heptylbenzene



Common Name: Heptylbenzene
Synonym: 1-phenylheptane
Chemical Name: $n$-heptylbenzene
CAS Registry No: 1078-71-3
Molecular Formula: $\mathrm{C}_{13} \mathrm{H}_{20}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{6} \mathrm{CH}_{3}$
Molecular Weight: 176.298
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-48 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 240 (Lide 2003)
Density (g/cm ${ }^{3}$ ): $0.8567 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$205.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
251.4 (calculated-Le Bas method at normal boiling point))

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
0.686; 0.925 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$133.3^{*} \quad\left(66.2^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $66.2-233^{\circ} \mathrm{C}$, Stull 1947)
1333* ( $112^{\circ} \mathrm{C}$, derived from compiled data, temp range $112-246^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0006-1761.2 /\left(181.5+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $112-279^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971) $\log (\mathrm{P} / \mathrm{kPa})=6.1255-[1761.2 /(\mathrm{T}-91.65)]$; temp range $423-527 \mathrm{~K}$ (liquid, Antoine equation, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=89.2811-6.4093 \times 10^{3} /(\mathrm{T} / \mathrm{K})-29.248 \cdot \log (\mathrm{~T} / \mathrm{K})+1.0328 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+6.2451 \times 10^{-14} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $225-714 \mathrm{~K}$ (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
5.768 (HPLC-k' correlation, Hanai \& Hubert 1981)
5.37 (HPLC-k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.27.1
Reported vapor pressures of heptylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(2) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K}) \quad$ (4)
Stull 1947
Zwolinski \& Wilhoit 1971

| summary of literature data |  | selected values |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 66.2 | 133.3 | 112 | 1333 | 243 | 94659 |
| 94.8 | 666.6 | 128 | 2666 | 243.6 | 95992 |
| 109 | 1333 | 137 | 4000 | 244.2 | 97325 |
| 124.2 | 2666 | 145 | 5333 | 244.8 | 98659 |
| 141.6 | 5333 | 150.7 | 6666 | 245.4 | 99992 |
| 151.5 | 7999 | 155.7 | 7999 | 246 | 101325 |
| 165.7 | 13332 | 164 | 10666 |  |  |
| 186.6 | 26664 | 170.7 | 13332 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 210 | 53329 | 183.6 | 19998 | A | 6.97833 |
| 233 | 101325 | 193.3 | 26664 | B | 1639.91 |
|  | - | 201.1 | 33331 | C | 194.76 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  | 207.8 | 39997 |  |  |
|  |  | 218.9 | 53329 | bp/ ${ }^{\circ} \mathrm{C}$ | 205.46 |
|  |  | 227.9 | 66661 | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
|  |  | 235.6 | 79993 | at $25^{\circ} \mathrm{C}$ | 55.06 |
|  |  | 242.3 | 93326 | at bp | 41.21 |



FIGURE 3.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for heptylbenzene.

### 3.1.1.28 $n$-Octylbenzene



Common Name: $n$-Octylbenzene
Synonym: 1-phenyloctane, octylbenzene
Chemical Name: $n$-octylbenzene
CAS Registry No: 2189-60-8
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{22}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{7} \mathrm{CH}_{3}$
Molecular Weight: 190.325
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-36 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
264 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ : $0.8582\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$222.2\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
273.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 29.96 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 127.91, 110.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.219; 0.204 (calculated-regression eq.; calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1333* $\quad\left(127^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $127-264.4^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0086-1812.2 /\left(174.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $127-298^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
7.666* $\quad\left(43^{\circ} \mathrm{C}\right.$, gas saturation, measured range $43-125.6^{\circ} \mathrm{C}$, Allemand et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=8.35571-3293.744 /(\mathrm{T} / \mathrm{K})$; temp range $368-400 \mathrm{~K}$ (liquid, Antoine equation, Stephenson \&
Malanowski 1987)
$1.15^{*} \quad\left(20.01^{\circ} \mathrm{C}\right.$, static method, measured range 293.16-462.87 K, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{kPa})=6.50210-2183.874 /\left(207.887+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $293.16-462.87 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=1.8919-4.1324 \times 10^{3} /(\mathrm{T} / \mathrm{K})+6.1473 \cdot \log (\mathrm{~T} / \mathrm{K})-2.0294 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+9.6879 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 237-729 K (Yaws 1994)
1.105* ( $20.34^{\circ} \mathrm{C}$, static method, measured range 293.49-462.87 K, Mokbel et al. 1998)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
6.30 (RP-TLC-RT correlation, Bruggeman et al. 1982)
6.52, 6.29 (RP-HPLC-k' correlation, Harnisch et al. 1982)
6.297 (HPLC-k' correlation, Hanai \& Hubert 1984)
6.35, 6.85 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
6.30 (recommended, Sangster 1993)
5.89 (HPLC-k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.28.1
Reported vapor pressures of octylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log P=A-B /(C+T / K)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4)

| Zwolinski \& Wilhoit 1971 |  | Allemand et al. 1986 |  | Kasehgari et al. 1993 |  | Mokbel et al. 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| selected values |  | gas saturation |  | static method |  | static method |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | T/K | $\mathbf{P / P a}$ | T/K | $\mathbf{P / P a}$ |
| 127 | 1333 | 43.0 | 7.666 | 293.16 | 1.15 | 293.49 | 1.105 |
| 143 | 2666 | 52.43 | 14.8 | 303.13 | 3.01 | 313.49 | 2.690 |
| 153 | 4000 | 72.75 | 66.8 | 313.01 | 6.87 | 303.48 | 6.316 |
| 161 | 5333 | 84.2 | 134.7 | 323.01 | 15.3 | 23.47 | 13.92 |
| 166.7 | 6666 | 95.39 | 262.7 | 333.15 | 31.5 | 333.48 | 28.76 |
| 171.9 | 7999 | 106.0 | 437.3 | 343.15 | 60.8 | 343.45 | 57.64 |
| 180.4 | 10666 | 125.64 | 1205 | 353.13 | 114 | 353.45 | 109.0 |
| 187.2 | 13332 |  |  | 363.14 | 207 | 363.42 | 198.0 |
| 200.3 | 19998 |  |  | 373.22 | 362 | 373.45 | 350.0 |
| 210.4 | 26664 |  |  | 383.25 | 609 | 403.00 | 1513 |
| 218.4 | 33331 |  |  | 393.32 | 994 | 412.96 | 2329 |
| 225.3 | 39997 |  |  | 403.33 | 1574 | 422.92 | 3504 |
| 236.7 | 53329 |  |  | 412.96 | 2329 | 432.94 | 5143 |
| 235.9 | 66661 |  |  | 422.92 | 3504 | 442.96 | 7395 |
| 253.8 | 79993 |  |  | 432.94 | 5143 | 452.90 | 10366 |
| 260.7 | 93326 |  |  | 442.96 | 7395 | 462.87 | 14266 |
| 261.9 | 95992 |  |  | 452.90 | 10370 |  |  |
| 263.2 | 98659 |  |  | 462.87 | 14270 | data fitt | Wagner eq. |

264.4101325

Antoine eq.

| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| :--- | :---: |
| A | 7.0086 |
| B | 1812.2 |
| C | 174.6 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 264.4 |
| $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |  |
| at $25^{\circ} \mathrm{C}$ | 69.96 |
| at bp | 46.9 |


| eq. 2 | $\mathrm{P} / \mathrm{kPa}$ |
| :---: | :---: |
| A | 6.50210 |
| B | 2183.874 |
| C | 207.887 |



FIGURE 3.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for octylbenzene.

### 3.1.1.29 Nonylbenzene



Common Name: Nonylbenzene
Synonym: 1-phenylnonane
Chemical Name: $n$-nonylbenzene
CAS Registry No: 1081-77-2
Molecular Formula: $\mathrm{C}_{15} \mathrm{H}_{24}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{8} \mathrm{CH}_{3}$
Molecular Weight: 204.352
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-24 (Dreisbach 1955; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
280.5 (Lide 2003)

Density (g/cm ${ }^{3}$ ): $0.8558,0.8522 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955) $0.8584 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
238.1 ( $20^{\circ} \mathrm{C}$, calculated-density)
295.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0725; 0.112 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.573 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.19041-1991.0 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $165-330^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ( $142^{\circ} \mathrm{C}$, derived from compiled data, temp range $142-282^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0245-1862.6 /\left(167.5+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $142-316^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
2.906* $\quad\left(43^{\circ} \mathrm{C}\right.$, gas saturation, measured range $43-142^{\circ} \mathrm{C}$, Allemand et al. 1986)
0.338 (GC-RT correlation, Sherblom et al. 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=-0.9235-4.2232 \times 10^{3} /(\mathrm{T} / \mathrm{K})+7.3073 \cdot \log (\mathrm{~T} / \mathrm{K})-2.0964 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+9.7152 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2}$, temp range $249-741 \mathrm{~K}$ (Yaws 1994)
$0.8747^{*} \quad\left(30.52^{\circ} \mathrm{C}\right.$, static method, measured range $313.67-466.46 \mathrm{~K}$, Mokbel et al. 1998)
Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
6.828 (HPLC-k' correlation, Hanai \& Hubert 1981)
6.83, 7.40 (RP-HPLC-k' correlations, Sherblom \& Eganhouse 1988)
7.11 (recommended, Sangster 1993)
6.41 (HPLC-k' correlation, Ritter et al. 1995)
6.83 (quoted from Sherblom \& Eganhouse 1988, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.29.1
Reported vapor pressures of nonylbenzene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| :--- | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |


| Zwolinski \& Wilhoit 1971 |  |  |  | Allemand et al. 1986 |  | Mokbel et al. 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| selected values |  |  |  | gas saturation |  | static method |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |  |  | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathbf{P / P a}$ |
| 142 | 1333 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 43 | 2.906 | 303.67 | 0.8474 |
| 158 | 2666 | A | 7.0245 | 50 | 5.186 | 313.65 | 2.271 |
| 168 | 4000 | B | 1862.6 | 59 | 10.36 | 323.67 | 5.369 |
| 176 | 5333 | C | 167.5 | 64 | 15.07 | 333.61 | 12.07 |
| 182.3 | 6666 |  |  | 74.32 | 31.73 | 343.53 | 25.20 |
| 187.5 | 7999 | bp/ ${ }^{\circ} \mathrm{C}$ | 282.0 | 85.0 | 64.26 | 351.83 | 44.97 |
| 196.2 | 10666 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ |  | 91.3 | 95.33 | 361.84 | 85.44 |
| 203.2 | 13332 | at $25^{\circ} \mathrm{C}$ | 74.81 | 98.28 | 146.7 | 371.75 | 155 |
| 216.7 | 19998 | at bp | 49.0 | 108.57 | 260.0 | 381.65 | 270 |
| 226.8 | 26664 |  |  | 120.0 | 480.0 | 391.62 | 459 |
| 235.1 | 33331 |  |  | 130.73 | 780.0 | 401.56 | 752 |
| 247.1 | 39997 |  |  | 142.0 | 1352 | 411.48 | 1207 |
| 253.7 | 53329 |  |  |  |  | 411.60 | 1203 |
| 263.1 | 66661 |  |  |  |  | 421.45 | 1881 |
| 271.1 | 79993 |  |  |  |  | 431.44 | 2835 |
| 278.2 | 93326 |  |  |  |  | 441.49 | 4201 |
| 279.5 | 95992 |  |  |  |  | 451.48 | 6053 |
| 280.7 | 98659 |  |  |  |  | 461.48 | 8591 |
| 282 | 101325 |  |  |  |  | 466.46 | 10099 |
|  |  |  |  |  |  | data fitted to Wagner eq. |  |



FIGURE 3.1.1.29.1 Logarithm of vapor pressure versus reciprocal temperature for nonylbenzene.

### 3.1.1.30 Decylbenzene



Common Name: Decylbenzene
Synonym: 1-phenyldecane
Chemical Name: $n$-decylbenzene
CAS Registry No: 104-72-3
Molecular Formula: $\mathrm{C}_{16} \mathrm{H}_{26}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{9} \mathrm{CH}_{3}$
Molecular Weight: 218.337
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-14.4 (Dreisbach 1955, Stephenson \& Malanowski 1987: Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
293 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ :
$0.85553,0.85189 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Camin et al. 1954; Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$255.3 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
318.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
2.50 (vapor-phase saturation, shake flask-GC, Sherblom et al. 1992)
5.59, 8.47, $10.55 \quad$ (calculated- $\mathrm{V}_{\mathrm{M}}, \mathrm{K}_{\mathrm{ow}}$, TSA, Sherblom et al. 1992)
0.023; 0.0188 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
8329* $\quad\left(202.987^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $202.987-297.799^{\circ} \mathrm{C}$, Camin et al. 1954)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03642-1904.132 /\left(160.318+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $202.9-297.9^{\circ} \mathrm{C}$ (Antoine eq., manometer measurements, Camin et al. 1954)
0.20 (extrapolated-Antoine eq., Dreisbach 1961)
$\log (\mathrm{P} / \mathrm{mmHg})=7.27177-2107.7 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $185-345^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ( $155.1^{\circ} \mathrm{C}$, derived from compiled data, temp range $155.1-297.89^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03642-1904.132 /\left(160.318+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $155.1-322.9^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{kPa})=6.16274-1905.56 /\left(160.503+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $203-297.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Camin et al. 1954, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=4.03653-876.208 /(\mathrm{T} / \mathrm{K}-203.15)$; temp range $317-427 \mathrm{~K}$ (liquid, Antoine equation, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{kPa})=6.15658-[1900.916 /(\mathrm{T} / \mathrm{K}-113.16)]$; temp range $475-571 \mathrm{~K}$ (liquid, Antoine equation, Stephenson \& Malanowski 1987)
0.133, $0.127\left(\mathrm{P}_{\mathrm{L}}, \mathrm{GC}-\mathrm{RT}\right.$ correlation, Sherblom et al. 1992)
0.707* $\quad\left(39.85^{\circ} \mathrm{C}\right.$, static method, measured range 313.0-433.23 K, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{kPa})=6.37655-2098.329 /\left(180.620+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $313.0-433.23 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=-4.4754-4.4669 \times 10^{3} /(\mathrm{T} / \mathrm{K})+9.1965 \cdot \log (\mathrm{~T} / \mathrm{K})-2.4010 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.0848 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 259-753 K (Yaws 1994)

Henry's Law Constant $\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right.$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
7.35 (RP-TLC retention time correlation, Bruggeman et al. 1982)
7.60, 7.33 (RP-HPLC-k' correlations, Harnisch et al. 1982)
7.358 (HPLC-k' correlation, Hanai \& Hubert 1984)
7.37, 8.01 (RP-HPLC-k' correlation, Sherblom \& Eganhouse 1988)
7.38 (HPLC-k' correlation, Sherblom et al. 1992)
7.35 (recommended, Sangster 1993)
6.94 (HPLC-k' correlation, Ritter et al. 1995)
7.37 (quoted from Sherblom \& Eganhouse 1988, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.30.1
Reported vapor pressures of decylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log P=A-B /(C+T / K)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K}) \quad$ (4)
Camin et al. $1954 \quad$ Zwolinski \& Wilhoit 1971

| ebulliometry |  | selected values |  |  |  | static method |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |  |  | T/K | $\mathbf{P / P a}$ |
| 202.987 | 8329 | 155.1 | 1333 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 313.0 | 0.797 |
| 211.392 | 10938 | 171.7 | 2666 | A | 7.03642 | 323.13 | 1.92 |
| 217.156 | 13088 | 182.19 | 4000 | B | 1904.132 | 343.15 | 10.3 |
| 230.476 | 19442 | 190.07 | 5333 | C | 160.318 | 353.11 | 21.6 |
| 244.331 | 28555 | 196.431 | 6666 |  |  | 363.12 | 41.9 |
| 260.372 | 43172 | 201.803 | 7999 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 297.89 | 373.25 | 78.5 |
| 278.950 | 67077 | 210.617 | 10666 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ | $\left.{ }^{-1}\right)=$ | 383.28 | 142 |
| 296.370 | 98146 | 217.755 | 13332 | at $25^{\circ} \mathrm{C}$ | 79.75 | 393.34 | 248 |
| 297.799 | 101113 | 231.452 | 19998 | at bp | 50.6 | 403.37 | 417 |
|  |  | 241.789 | 26664 |  |  | 413.33 | 683 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 297.083 | 250.19 | 33331 |  |  | 413.33 | 684 |
|  |  | 257.18 | 39997 |  |  | 423.21 | 1081 |
|  |  | 269.86 | 53329 |  |  | 433.23 | 1687 |
|  |  | 278.68 | 66661 |  |  |  |  |
|  |  | 286.843 | 79993 |  |  | Antoine eq |  |
|  |  | 293.986 | 93326 |  |  | eq. 2 | $\mathrm{P} / \mathrm{kPa}$ |
|  |  | 295.969 | 95992 |  |  | A | 6.37655 |
|  |  | 296.616 | 98659 |  |  | B | 2098.329 |
|  |  | 297.89 | 101325 |  |  | C | 180.620 |



FIGURE 3.1.1.30.1 Logarithm of vapor pressure versus reciprocal temperature for decylbenzene.

### 3.1.1.31 Undecylbenzene



Common Name: Undecylbenzene
Synonym: 1-phenylundecane
Chemical Name: $n$-undecylbenzene
CAS Registry No: 6742-54-7
Molecular formula: $\mathrm{C}_{17} \mathrm{H}_{28}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{10} \mathrm{CH}_{3}$
Molecular Weight: 232.404
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-5.0 (Dreisbach 1955; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
316 (Dreisbach 1955; Lide 2003)
Density (g/cm ${ }^{3}$ ):
0.8553, $0.8517 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1961)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$271.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
340.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ): 0.00702; 0.00377 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.080 (calculated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.34672-2215.1 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $195-375^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* $\quad\left(168^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $168-313.2^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0509-1944.1 /\left(153.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $168-349^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971) $0.050,0.047 \quad\left(\mathrm{P}_{\mathrm{L}}\right.$, GC-RT correlation, Sherblom et al. 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=124.1549-8.8970 \times 10^{3} /(\mathrm{T} / \mathrm{K})-41.223 \cdot \log (\mathrm{~T} / \mathrm{K})+1.3662 \times 10^{-2} .(\mathrm{T} / \mathrm{K})-8.1321 \times 10^{-14} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 268 - 764 K (Yaws 1994)
$0.7156^{*} \quad\left(50.42^{\circ} \mathrm{C}\right.$, static method, measured range $323.57-467.33^{\circ} \mathrm{C}$, data fitted to Wagner eq., Mokbel et al. 1998)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
8.14 (RP-HPLC-RT correlation, Sherblom et al. 1992, quoted, Sangster 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.31.1
Reported vapor pressures of undecylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
Zwolinski \& Wilhoit 1971
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$

Mokbel et al. 1998

| selected values |  |  |  | static method |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | T/K | $\mathbf{P / P a}$ | T/K | P/Pa |
| 168 | 1333 | 309.2 | 93326 | 323.57 | 0.7156 | 462.28 | 3088 |
| 185 | 2666 | 310.6 | 95992 | 333.59 | 1.820 | 467.33 | 37726 |
| 196 | 4000 | 311.9 | 98659 | 343.71 | 4.304 |  |  |
| 204 | 5333 | 313.2 | 101325 | 352.69 | 9.405 | data fi | Wagner eq. |
| 210.3 | 6666 |  |  | 363.78 | 19.39 |  |  |
| 215.7 | 7999 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 372.07 | 34.36 |  |  |
| 224.7 | 10666 | A | 7.0590 | 382.06 | 64.41 |  |  |
| 231.9 | 13332 | B | 1944.1 | 392.06 | 117 |  |  |
| 245.8 | 19998 | C | 153.0 | 402.11 | 204 |  |  |
| 256.3 | 26664 |  |  | 412.11 | 344 |  |  |
| 264.8 | 33331 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 313.2 | 422.09 | 564 |  |  |
| 272.1 | 39997 |  | $\left.\mathrm{mol}^{-1}\right)=$ | 422.19 | 568 |  |  |
| 284 | 53329 | at $25^{\circ} \mathrm{C}$ | 84.68 | 432.25 | 908 |  |  |
| 293.7 | 66661 | at bp | 52.3 | 442.27 | 1369 |  |  |
| 302 | 79993 |  |  | 452.29 | 2080 |  |  |



FIGURE 3.1.1.31.1 Logarithm of vapor pressure versus reciprocal temperature for undecylbenzene.

### 3.1.1.32 Dodecylbenzene



Common Name: Dodecylbenzene
Synonym: 1-phenyldodecane
Chemical Name: $n$-dodecylbenzene
CAS Registry No: 123-01-3
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{30}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{11} \mathrm{CH}_{3}$
Molecular Weight: 246.431
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
$3.0 \quad$ (Dreisbach 1955; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
328 (Lide 2003)
Density (g/cm ${ }^{3}$ ): $0.8551,0.8516 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
288.2 ( $20^{\circ} \mathrm{C}$, calculated-density)
362.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
26.66* $\quad\left(78.4^{\circ} \mathrm{C}\right.$, ebulliometry-McLeod gauge, measured range $78.4-288.6^{\circ} \mathrm{C}$, Myers \& Fenske 1955)
0.032 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.41934-2319.2 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $210-385^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

1333* ( $181^{\circ} \mathrm{C}$, derived from compiled data, temp range $181-327.6^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971) $\log (\mathrm{P} / \mathrm{mmHg})=7.0693-1981.6 /\left(145.5+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $181-363^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971) 1.08* ( $53.7^{\circ} \mathrm{C}$, gas saturation, measured range $53.7-192.7^{\circ} \mathrm{C}$, Allemand et al. 1986) $0.019,0.017$ ( $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation, Sherblom et al. 1992) 0.727* ( $69.771^{\circ} \mathrm{C}$, static method, measured range 332.92-453.26 K, Kasehgari et al. 1993) $\log (\mathrm{P} / \mathrm{kPa})=6.66087-2371.902 /\left(182.311+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $332.92-453.26 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=145.6916-1.0165 \times 10^{3} /(\mathrm{T} / \mathrm{K})-48.761 \cdot \log (\mathrm{~T} / \mathrm{K})+1.5985 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+4.881 \times 10^{-13} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 276 - 774 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
8.65 (RP-HPLC-k' correlation, Sherblom et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.32.1
Reported vapor pressures of dodecylbenzene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| Myers \& Fenske 1955 |  | Zwolinski \& Wilhoit 1971 |  | Allemand et al. 1986 |  | Kasehgari et al. 1993 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometryMcLeod gauge |  | selected values |  | gas saturation |  | static method |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | $\mathbf{P / P a}$ |
| 78.4 | 26.66 | 181 | 1333 | 53.7 | 1.080 | 343.21 | 0.640 |
| 91.2 | 66.66 | 198 | 2666 | 86.19 | 6.733 | 353.26 | 1.61 |
| 102.3 | 133.3 | 209 | 4000 | 93.0 | 11.15 | 363.23 | 3.72 |
| 114.2 | 266.6 | 217 | 5333 | 103.0 | 21.60 | 363.23 | 3.73 |
| 122.4 | 400.0 | 223.5 | 6666 | 111.0 | 36.40 | 373.21 | 8.11 |
| 128.2 | 533.3 | 229.0 | 7999 | 124.02 | 79.86 | 383.22 | 16.9 |
| 133.4 | 666.6 | 238.1 | 10666 | 136.47 | 158.7 | 393.22 | 32.8 |
| 137.0 | 800 | 245.4 | 13332 | 160.44 | 540 | 403.27 | 59.5 |
| 143.5 | 1067 | 259.5 | 19998 | 192.71 | 1464 | 413.28 | 106 |
| 148.8 | 1333 | 270.1 | 26664 |  |  | 423.29 | 182 |
| 158.5 | 2000 | 278.7 | 33331 |  |  | 433.37 | 306 |
| 165,6 | 2666 | 286 | 39997 |  |  | 443.39 | 493 |
| 176.4 | 4000 | 298.1 | 53329 |  |  | 453.33 | 760 |
| 184.2 | 5333 | 307.9 | 66661 |  |  | 463.38 | 1167 |
| 191.0 | 6666 | 316.3 | 79993 |  |  |  |  |
| 196.0 | 7999 | 323.6 | 93326 |  |  |  | ne eq |
| 205.5 | 10666 | 325 | 95992 |  |  | eq. 2 | $\mathrm{P} / \mathrm{kPa}$ |
| 212.0 | 13332 | 326.3 | 98659 |  |  | A | 6.66087 |
| 225.4 | 19998 | 327.6 | 101325 |  |  | B | 2371.902 |
| 235.8 | 26664 |  |  |  |  | C | 182.311 |
| 250.3 | 39997 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |
| 262.0 | 53329 | A | 7.0693 |  |  |  |  |
| 270.4 | 66661 | B | 1981.6 |  |  |  |  |
| 278.2 | 79992 | C | 145.5 |  |  |  |  |
| 285.5 | 93326 |  |  |  |  |  |  |
| 288.6 | 101325 | bp/ ${ }^{\circ} \mathrm{C}$ | 327.6 |  |  |  |  |
|  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |  |  |  |  |  |
|  |  | at $25^{\circ} \mathrm{C}$ | 89.62 |  |  |  |  |
|  |  | at bp | 54.4 |  |  |  |  |



FIGURE 3.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for dodecylbenzene.

### 3.1.1.33 Tridecylbenzene



Common Name: Tridecylbenzene
Synonym: 1-phenyltridecane
Chemical Name: n-tridecylbenzene
CAS Registry No: 123-02-4
Molecular Formula: $\mathrm{C}_{19} \mathrm{H}_{32}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{12} \mathrm{CH}_{3}$
Molecular Weight: 260.457
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
10 (Dreisbach 1955; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
346 (Dreisbach 1955; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ :
$0.8550,0.8515 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$304.6 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
384.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ : 0.233 (vapor saturation-shake flask-GC, Sherblom et al. 1992)
$0.233,0.0885,0.181$ (calculated $-\mathrm{V}_{\mathrm{m}}, \mathrm{K}_{\mathrm{OW}}$, TSA, Sherblom et al. 1992)
0.00067 ; 0.00137 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.0125 (extrapolated-Antoine eq., Dreisbach 1955) $\log (\mathrm{P} / \mathrm{mmHg})=7.49437-2626.7 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $226-405^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955) 1333* $\quad\left(193^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $193-341.2^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971) $\log (\mathrm{P} / \mathrm{mmHg})=7.0843-2013.9 /\left(137.9+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $193-376^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971) $0.008,0.07$ ( $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation, Sherblom et al. 1992)
$0.64^{*} \quad\left(70.06^{\circ} \mathrm{C}\right.$, static method, measured range 343.21-463.38 K, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{kPa})=6.13410-2087.968 /\left(153.790+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $343.21-463.38 \mathrm{~K}$ (static method, Kasehgari et al. 1993)
$\log (\mathrm{P} / \mathrm{mmHg})=160.3924-1.1093 \times 10^{4} /(\mathrm{T} / \mathrm{K})-53.875 \cdot \log (\mathrm{~T} / \mathrm{K})+1.7532 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+3.727 \times 10^{-13} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $283-783 \mathrm{~K}$ (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
9.36 (RP-HPLC-k' correlation, Sherblom et al. 1992)
8.97; 8.54 (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.33.1
Reported vapor pressures of tridecylbenzene at various temperatures
Zwolinski \& Wilhoit 1971

| selected values |  |  |  | static method |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| 193 | 1333 | 338.5 | 95992 | 343.20 | $6.40 \times 10^{-4}$ |
| 210 | 2666 | 339.9 | 98659 | 353.26 | $1.61 \times 10^{-3}$ |
| 221 | 4000 | 341.2 | 101325 | 363.23 | $3.73 \times 10^{-3}$ |
| 229 | 5333 |  |  | 373.21 | $8.11 \times 10^{-3}$ |
| 236 | 6666 | $\log \mathrm{P}$ | B/(C $\left.+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | 383.22 | 0.0169 |
| 242 | 7999 |  | $\mathrm{P} / \mathrm{mmHg}$ | 393.22 | 0.0328 |
| 251 | 10666 | A | 7.0843 | 403.27 | 0.0595 |
| 258.2 | 13332 | B | 2013.9 | 413.28 | 0.106 |
| 271.6 | 19998 | C | 137.9 | 423.29 | 0.182 |
| 283.1 | 26664 |  |  | 433.37 | 0.306 |
| 291.8 | 33331 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 341.2 | 443.39 | 0.493 |
| 299.2 | 39997 | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}$ |  | 453.33 | 0.760 |
| 311.4 | 53329 | at $25^{\circ} \mathrm{C}$ | 94.6 | 463.38 | 1.167 |
| 321.3 | 66661 | at bp | 56.1 |  |  |
| 329.8 | 79993 |  |  |  |  |
| 337.2 | 93326 |  |  |  |  |

### 3.1.1.34 Tetradecylbenzene



Common Name: Tetradecylbenzene
Synonym: 1-phenyltetradecane
Chemical Name: $n$-tetradecylbenzene
CAS Registry No: 1459-10-5
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{34}, \mathrm{C}_{6} \mathrm{H}_{5}\left(\mathrm{CH}_{2}\right)_{13} \mathrm{CH}_{3}$
Molecular Weight: 274.484
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
16 (Dreisbach 1955; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
359 (Dreisbach 1955; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
$0.8549,0.8514 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$321.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
406.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$ are compiled at the end of this section):
1333* $\quad\left(205^{\circ} \mathrm{C}\right.$, derived from compiled data, temp range $205-354^{\circ} \mathrm{C}$, Zwolinski \& Wilhoit 1971$)$ 0.0055 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Sherblom et al. 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.56143-2522.8 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $235-410^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.101-2042 /\left(130+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $205-300^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971) $0.002 \quad\left(\mathrm{P}_{\mathrm{L}}\right.$, GC-RT correlation, Sherblom et al. 1992)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
9.95 (RP-HPLC-k' correlation, Sherblom et al. 1992)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

## TABLE 3.1.1.34.1

Reported vapor pressures of tetradecylbenzene at various temperatures
Zwolinski \& Wilhoit 1971

| selected values |  |  |  |
| :---: | :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 205 | 1333 | 351 | 95992 |
| 222 | 2666 | 353 | 98659 |
| 233 | 4000 | 354 | 101325 |
| 241 | 5333 |  |  |
| 248 | 6666 |  | $\operatorname{log~P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| 254 | 7999 | $\mathrm{eq} 2$. | $\mathrm{P} / \mathrm{mmHg}$ |
| 263 | 10666 | A | 7.010 |
| 270 | 13332 | B | 2042.0 |
| 285 | 19998 | C | 130.0 |
| 295 | 26664 |  |  |
| 304 | 33331 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 354.0 |
| 312 | 39997 | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}{ }^{-1}\right)$ |  |
| 324 | 53329 | at $25^{\circ} \mathrm{C}$ | 99.6 |
| 334 | 66661 | at bp | 57.7 |
| 342 | 79993 |  |  |
| 350 | 93326 |  |  |

### 3.1.1.35 Styrene



Common Name: Styrene
Synonym: phenylethene, styrol, styrolene cinnamene, cinnamol, phenylethylene, vinylbenzene, ethenylbenzene
Chemical Name: styrene
CAS Registry No: 100-42-5
Molecular Formula: $\mathrm{C}_{8} \mathrm{H}_{8}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 104.150
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-30.65 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 145 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.9060, $0.9012 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach \& Martin 1949; Dreisbach 1955; Riddick et al. 1986)
0.906 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$115.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
133.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 43.932, $38.7\left(25^{\circ} \mathrm{C}\right.$, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 10.95 (Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 45.15, 52.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$330^{*} \quad\left(24^{\circ} \mathrm{C}\right.$, shake flask-Karl Fischer titration, measured range $7-51^{\circ} \mathrm{C}$, Lane 1946)
310* (cloud point method, measured range $10-60^{\circ} \mathrm{C}$, Lane 1946)
220 (shake flask-method not specified, Frilette \& Hohenstein 1948)
300 (shake flask-UV, Andrews \& Keefer 1950)
160 (shake flask-HPLC/UV, Banerjee et al. 1980)
250* (recommended best value, temp range $10-60^{\circ} \mathrm{C}$, Shaw 1989b)
$\ln x=-19.471-1655.9 /(\mathrm{T} / \mathrm{K})-4.6244 \times 10^{-5} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
288* $\quad\left(8.2^{\circ} \mathrm{C}\right.$, mercury manometer, measured range -7.7 to $8.2^{\circ} \mathrm{C}$, Linder 1931)
$\log (\mathrm{P} / \mathrm{mmHg})=7.929-2103 /(\mathrm{T} / \mathrm{K})$; temp range $33.5-116.3^{\circ} \mathrm{C}$ (isoteniscope method, Burchfield 1942)
841.3* (static-Hg manometer, measured range $12.5-60^{\circ} \mathrm{C}$, Pitzer et al. 1946)
969.4* (calculated-Antoine eq. regression, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=7.22302-1629.2 /\left(230+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ (Antoine eq., Dreisbach \& Martin 1949)
$6799^{*} \quad\left(66.7^{\circ} \mathrm{C}\right.$, mercury manometer, Buck et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=-3151 /(\mathrm{T} / \mathrm{K})-6.294 \cdot \log (\mathrm{~T} / \mathrm{K})+26.92$; temp range $80-120^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
807 (extrapolated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92409-1430.0 /\left(206.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $55-205^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1093* $\quad\left(29.92^{\circ} \mathrm{C}\right.$, measured range $29.92-110.06^{\circ} \mathrm{C}$, Dreyer et al. 1955)
1333* $\quad\left(32.24^{\circ} \mathrm{C}\right.$, measured range $32.4-82.9^{\circ} \mathrm{C}$, Chaiyavech \& van Winkle 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=8.2696-2221.21 /(\mathrm{T} / \mathrm{K})$; temp range $32.4-82.9^{\circ} \mathrm{C}$ (Chaiyavech \& van Winkle 1959)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 9634.7 /(\mathrm{T} / \mathrm{K})]+7.922049$; temp range -7.0 to $145.2^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
879, 812 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.14016-1574.511 /\left(224.087+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32.4-62.19^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.06623-1507.434 /\left(214.985+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $29.92-144.77^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{atm})=(1-418.675 / \mathrm{T}) \times 10^{\wedge}\left(0.886470-8.14267 \times 10^{4} \cdot \mathrm{~T}+7.57896 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 281.35-417.92 K (Cox vapor pressure eq., Chao et al. 1983)

878, 811 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.235-1557.406 /(222.538+\mathrm{T} / \mathrm{K})$; temp range $32.4-62.19^{\circ} \mathrm{C}$ (Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.18301-1501.162 /\left(214.42+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $29.92-144.77^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
879 (extrapolated, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.14016-1774.51 /\left(224.09+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32-82^{\circ} \mathrm{C}$ (Antoine eq., Dean, 1985, 1992)
841 (lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=6.34792-1629.20 /\left(230.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range not specified (Antoine eq., Riddick et al. 1986)
880 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.3945-2221.3 /(\mathrm{T} / \mathrm{K})$; temp range $245-334 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.08201-1445.58 /(-63.72+\mathrm{T} / \mathrm{K})$; temp range $334-419 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=55.8621-4.024 \times 10^{3} /(\mathrm{T} / \mathrm{K})-17.609 \cdot \log (\mathrm{~T} / \mathrm{K})+6.6842 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.9438 \times 10^{-13} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 243-648 K (Yaws 1994)
$\log (\mathrm{P} / \mathrm{kPa})=7.3945-2221.3 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
233 (calculated-P/C, Mackay \& Shiu 1990)
285, 527 (quoted, Howard et al. 1989)
267 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
297 (exponential saturator EXPSAT technique, Dohnal \& Hovorka 1999)
$261\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimental determined values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=5.628-1935 /(\mathrm{T} / \mathrm{K})$ (summary of literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.14 (calculated-fragment const., Rekker 1977)
2.95 (shake flask, Hansch \& Leo 1979)
3.16 (shake flask-HPLC, Banerjee et al. 1980)
2.76 (HPLC-RT correlation Fujisawa \& Masuhara 1981)
2.90 (HPLC-RT correlation, Wang et al. 1986)
3.05 (recommended, Sangster 1989, 1993)
2.95 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
1.13 (goldfish, Ogata et al. 1984)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.42-2.74 (Swann et al. 1983)
2.96, 2.71 (quoted exptl., calculated-MCI $\chi$, Meylan et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: Volatilization and biodegradation may be dominant transport and transformation processes for styrene in water; calculated volatilization $t_{1 / 2}=3 \mathrm{~h}$ from a river $1-\mathrm{m}$ deep with a current speed of $1.0 \mathrm{~m} / \mathrm{s}$ and wind velocity of $3 \mathrm{~m} / \mathrm{s}$ (Howard 1989);
volatilized rapidly from shallow layers of lake water with $t_{1 / 2}=1$ to 3 h , but much slower from soil (Fu \& Alexander 1992).
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O} 3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{O} 3}=1.8 \times 10^{4} \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with ozone at $30^{\circ} \mathrm{C}$ (Bufalini \& Altshuller 1965)
$\mathrm{k}_{\mathrm{O} 3}=(22.6 \pm 4.6) \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=5.25 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson 1985)
$\mathrm{k}_{\mathrm{O} 3}=22 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=(5.87 \pm 0.15) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=(1.51 \pm 0.2) \times 10^{-13}$
$\mathrm{cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (Atkinson \& Aschmann 1988)
$\mathrm{k}_{\mathrm{OH}}=5.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{O} 3}=1.71 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Tuazon et al. 1993)
Hydrolysis: no hydrolyzable groups (Howard et al. 1991).
Biodegradation: $\mathrm{t}_{1 / 2}$ (aerobic) $=336-672 \mathrm{~h}$, based on unacclimated grab samples of aerobic soil and a subsurface sample; $\mathrm{t}_{1 / 2}($ anaerobic $)=1344-2688 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
styrene will be rapidly destroyed by biodegradation in most aerobic environments, and the rate may be slow at low concentrations in aquifers and lake waters and in environments at low pH ( $\mathrm{Fu} \&$ Alexander 1992) $\mathrm{t}_{1 / 2}($ aerobic $)=14 \mathrm{~d}, \mathrm{t}_{1 / 2}=56 \mathrm{~d}$ in natural waters $($ Capel \& Larson 1995)
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: atmospheric $t_{1 / 2} \sim 2.4-24 \mathrm{~h}$, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); will react rapidly with both hydroxyl radical and ozone in air with a combined $\mathrm{t}_{1 / 2}(\mathrm{calc})=2.5 \mathrm{~h}$, the reaction $\mathrm{t}_{1 / 2}=3.5 \mathrm{~h}$ with OH radicals and $\mathrm{t}_{1 / 2}=9 \mathrm{~h}$ with ozone (Howard 1989);
photooxidation $\mathrm{t}_{1 / 2}=0.9$ to 7.3 h , based on measured rate data for the reaction with OH radical and $\mathrm{O}_{3}$ in air (Howard et al. 1991);
calculated lifetimes of styrene due to reaction with OH radicals, $\mathrm{NO}_{3}$ radicals and $\mathrm{O}_{3}$ are $\sim 3 \mathrm{~h}, \sim 4 \mathrm{~h}$ and 1 d , respectively, for ambient atmospheric conditions (Tuazon et al. 1993);
calculated lifetimes of $1.4 \mathrm{~h}, 3.7 \mathrm{~h}$ and 1.0 d for reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$ respectively (Atkinson 2000).
Surface water: $\mathrm{t}_{1 / 2}=0.6 \mathrm{~d}$ in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)
$t_{1 / 2}=336-672 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$t_{1 / 2}($ calc $)=0.75-51 \mathrm{~d}$ for styrene loss from surface waters (Fu \& Alexander 1992).
Ground water: $t_{1 / 2}=672-5040 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life and acclimated aqueous screening test data (Howard et al. 1991).
Sediment:
Soil: $\mathrm{t}_{1 / 2}=336-672 \mathrm{~h}$, based on unacclimated grab samples of aerobic soil and acclimated aqueous screening test data (Howard et al. 1991).
Biota:

TABLE 3.1.1.35.1
Reported aqueous solubilities of styrene at various temperatures

| Lane 1946 |  |  |  | Shaw 1989b (IUPAC) recommended values |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-titration |  | shake flask-cloud pt. |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 7 | 290 | 15 | 250 | 10 | 290 |
| 24 | 330 | 25 | 310 | 20 | 300 |
| 32 | 360 | 44 | 400 | 25 | 340 |
| 40 | 400 | 49 | 450 | 30 | 340 |
| 51 | 450 | 65 | 500 | 40 | 400 |
|  |  |  |  | 50 | 460 |
|  |  |  |  | 60 | 530 |



FIGURE 3.1.1.35.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for styrene.

TABLE 3.1.1.35.2
Reported vapor pressures of styrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
1.

| Linder 1931 | Pitzer et al. 1946 |  | Stull 1947 |  | Buck et al. 1949 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Hg manometer | static-Hg manometer |  | summary of literature data |  | Hg manometer |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -7.7 86.66 | 12.5 | 384 | -7.0 | 133.3 | 66.7 | 6799 |
| -0.5 105.7 | 25 | 841.3 | 18 | 666.6 | 75.4 | 9866 |
| 8.2288 | 37.5 | 1692 | 30.8 | 1333 | 82.4 | 13332 |
|  | 50 | 3230 | 44.6 | 2666 | 88 | 16665 |
|  | 60 | 5177 | 59.8 | 5333 | 91.7 | 18932 |
| Burchfield 1942 |  |  | 69.5 | 7999 | 95.1 | 21732 |
| isoteniscope method | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -30.68 | 82 | 13332 | 98.2 | 24665 |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ |  |  | 101.3 | 26664 | 119.1 | 48129 |
|  | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 122.5 | 53329 | 132.6 | 71461 |
| data presented by | A | 28.8631 | 145.2 | 101325 | 145 | 100658 |
| Clausius-Clapeyron eq. | B | 3203 |  |  |  |  |
|  | C | 7 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -30.6 |  |  |
| eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ |  |  |  |  | eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ |
| A 7.929 | $\Delta \mathrm{H}_{\text {fus }}\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=10.95$ |  |  |  | A | 26.92 |
| B 2103 |  |  |  |  | B | 3151 |
| measured temp range: | $\Delta \mathrm{H}_{\mathrm{V}}\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=43.93$ |  |  |  | C | 6.294 |
| $33.5-116.3^{\circ} \mathrm{C}$ | at $25^{\circ} \mathrm{C}$ |  |  |  |  |  |

2. 

Dreyer et al. 1955
Chaiyavech \& Van Winkle 1959

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :--- | :---: | :---: | :---: | :---: |
| 29.92 | 1093 |  | 32.4 | 1333 |
| 39.21 | 1827 |  | 35.6 | 2666 |
| 60.04 | 5106 |  | 53.86 | 4000 |
| 74.42 | 9639 |  | 60.05 | 5333 |
| 85.53 | 14999 |  | 65.45 | 6666 |
| 99.51 | 25105 |  | 76.6 | 10666 |
| 110.06 | 56877 |  | 82.9 | 13332 |
|  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |  |
|  |  | A | 8.2696 |  |
|  |  | B | 2221.3 |  |



FIGURE 3.1.1.35.2 Logarithm of vapor pressure versus reciprocal temperature for styrene.

### 3.1.1.36 $\alpha$-Methylstyrene



Common Name: $\alpha$-Methylstyrene Synonym: isopropenylbenzene Chemical Name: $\alpha$-Methylstyrene CAS Registry No: 98-83-9
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{10}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{C}\left(\mathrm{CH}_{3}\right)=\mathrm{CH}_{2}$
Molecular Weight: 118.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-23.2 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
165.4 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ : $0.9106,0.9062 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955) $0.9082 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$129.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 11.92 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 47.55, 53.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$133.3^{*} \quad\left(7.4^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $7.4-165.4^{\circ} \mathrm{C}$, Stull 1947) $\log (\mathrm{P} / \mathrm{mmHg})=7.28240-1740.3 /\left(230+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)($ Antoine eq., Dreisbach \& Martin 1949) 333 (extrapolated by formula., Dreisbach 1855)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92366-1486.88 /\left(202.4+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $70-220^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10214.6 /(\mathrm{T} / \mathrm{K})]+7.959753$; temp range $7.4-165.4^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73) $\log (\mathrm{P} / \mathrm{mmHg})=6.92366-1486.88 /\left(202.4+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Dean 1985, 1992) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.04856-1486.88 /(-70.75+\mathrm{T} / \mathrm{K})$; temp range $343-493 \mathrm{~K}$ (liquid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.294-1599.88 /(-63.72+\mathrm{T} / \mathrm{K})$; temp range $353-413 \mathrm{~K}$ (liquid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-0.8626-2.5638 \times 10^{3} /(\mathrm{T} / \mathrm{K})+5.3807 \cdot \log (\mathrm{~T} / \mathrm{K})-1.3516 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+6.7181 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $250-654 \mathrm{~K}$ (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.48 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Photooxidation: $\mathrm{k}=(52 \pm 6) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the gas-phase reactions with OH radical at $298 \pm 2 \mathrm{~K}$ (Atkinson 1989).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:

## TABLE 3.1.1.36.1

Reported vapor pressures of $\alpha$-methylstyrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

$$
\begin{align*}
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1}\\
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) \tag{1a}
\end{align*}
$$

$\log P=A-B /(T / K)-C \cdot \log (T / K)$
Stull 1947

| summary of literature data |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 7.4 | 133.3 |
| 34.0 | 666.6 |
| 47.1 | 1333 |
| 61.8 | 2666 |
| 77.8 | 5333 |
| 88.3 | 7999 |
| 102.2 | 13332 |
| 121.8 | 26664 |
| 143 | 53329 |
| 165.4 | 101325 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -23.2 |



FIGURE 3.1.1.36.1 Logarithm of vapor pressure versus reciprocal temperature for $\alpha$-methylstyrene.

### 3.1.1.37 $\beta$-Methylstyrene



Common Name: $\beta$-Methylstyrene
Synonym: propenylbenzene
Chemical Name: $\beta$-Methylstyrene
CAS Registry No: 766-90-5 (cis-); 873-66-5 (trans-)
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{10}, \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}=\mathrm{CHCH}_{3}$
Molecular Weight: 118.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-61.6 (cis-, Stephenson \& Malanowski 1987; Lide 2003)
-29.3 (trans-, Stephenson \& Malanowski 1987; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
174 (cis-, Stephenson \& Malanowski 1987)
175-176 (trans-, Stephenson \& Malanowski 1987)
167.5 (cis-, Lide 2003)
178.3 (trans-, Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right)$ :
$0.9088 \quad\left(20^{\circ} \mathrm{C}\right.$, cis-, Lide 2003)
$0.9023 \quad\left(25^{\circ} \mathrm{C}\right.$, trans-, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
129.7 (cis-, Stephenson \& Malanowski 1987)
131.0 (trans-, Stephenson \& Malanowski 1987)
155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ}$ C, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* ( $17.5^{\circ} \mathrm{C}$, summary of literature data, measured range $32.1-112^{\circ} \mathrm{C}$, temp range $17.5-179^{\circ} \mathrm{C}$, Stull 1947 ) 267 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.92339-1499.80 /\left(201.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-200^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10701.3 /(\mathrm{T} / \mathrm{K})]+8.071487 ;$ temp range $17.5-179^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) $\log (\mathrm{P} / \mathrm{mmHg})=6.92339-1499.80 /\left(201.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range not specified (Antoine eq., Dean 1985, 1992) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.04829-1499.8 /(-72.15+\mathrm{T} / \mathrm{K})$; temp range $348-498 \mathrm{~K}$ (cis-, liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.58873-1915.94 /(-33.996+\mathrm{T} / \mathrm{K})$; temp range 291-452 K (trans-, liquid, Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :

Environmental Fate Rate Constant and Half-Lives:
Volatilization:
Photolysis:
Photooxidation: rate constant $\mathrm{k}=(59 \pm 6) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for the gas-phase reactions with OH radical at $298 \pm 2 \mathrm{~K}$ (Atkinson 1989)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
Half-Lives in the Environment:

TABLE 3.1.1.37.1
Reported vapor pressures of $ß$ methylstyrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
Stull 1947
summary of literature data

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :--- | :---: |
| 17.5 | 133.3 |
| 43.8 | 666.6 |
| 57 | 1333 |
| 71.5 | 2666 |
| 87.7 | 5333 |
| 97.8 | 7999 |
| 111.7 | 13332 |
| 132 | 26664 |
| 154.7 | 53329 |
| 179.0 | 101325 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -30.1 |



FIGURE 3.1.1.37.1 Logarithm of vapor pressure versus reciprocal temperature for $\beta$-methylstyrene.

### 3.1.1.38 o-Methylstyrene



Common Name: o-Methylstyrene
Synonym: 2-methylstyrene, 2-vinyl toluene, o-methylvinylbenzene
Chemical Name: 2-methylstyrene
CAS Registry No: 611-15-4
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{10}, 2-\mathrm{CH}_{3} \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 118.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-68.5 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
$169.8 \quad$ (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ): $0.9106 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$129.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
387* $\quad\left(32.1^{\circ} \mathrm{C}\right.$, differential manometer, measured range $32.1-112^{\circ} \mathrm{C}$, Clements et al. 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=7.15212-1628.405 /\left(211.386+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $32.1-112^{\circ} \mathrm{C}$ (Antoine eq. from differential manometer measurements, Clements et al. 1953)
240.8 (extrapolated-Antoine eq., Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.09235-1582.7 /\left(206.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-200^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
298.9 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.21287-1644.083 /\left(214.585+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32-112.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{atm})=\left(1-443.504 /(\mathrm{T} / \mathrm{K}) \times 10^{\wedge}\left[0.890379-7.17666 \times 10^{4} \cdot(\mathrm{~T} / \mathrm{K})+5.97058 \times 10^{7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right] ;\right.$ temp range
305.16-385.5 K (Cox vapor pressure eq., Chao et al. 1983)
246.4 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.33107-1660.041 /\left(214.219+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32-112.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.2129-1644.08 /\left(214.59+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $32-112^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.88461-1485.41 /\left(200.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-255^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.27762-1628.405 /(-61.764+\mathrm{T} / \mathrm{K})$; temp range $305-385 \mathrm{~K}$ (liquid, Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=36.8413-3.7269 \times 10^{3} /(\mathrm{T} / \mathrm{K})-9.7997 \cdot \log (\mathrm{~T} / \mathrm{K})+1.4115 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+1.9658 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range 205-659 K (Yaws 1994)

Henry's Law Constant (Pa•m³mol):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.38.1
Reported vapor pressures of omethylstyrene at various temperatures

Clements et al. 1953

|  | differential manometer |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 32.01 | 387 |
| 40.85 | 663 |
| 58.51 | 1753 |
| 58.54 | 1765 |
| 70.2 | 3113 |
| 82.8 | 5529 |
| 82.83 | 5534 |
| 100.35 | 11310 |
| 12.35 | 17698 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -68.57 |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 169.8 |
|  | $\Delta \mathrm{H}_{\mathrm{V}}=35.54 \mathrm{~kJ} / \mathrm{mol}$ |
|  | $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| eq. 2 | mmHg |
| A | 7.15272 |
| B | 1628.405 |
| C | 211.386 |



FIGURE 3.1.1.38.1 Logarithm of vapor pressure versus reciprocal temperature for o-methylstyrene.

### 3.1.1.39 m-Methylstyrene



Common Name: $m$-Methylstyrene
Synonym: methylvinylbenzene, 3-vinyl toluene, $m$-methylvinylbenzene
Chemical Name: 3-methylstyrene
CAS Registry No: 100-42-1
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{10}, 3-\mathrm{CH}_{3} \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 118.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-86.3 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
164 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : $0.9028 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $130.9 \quad\left(\left(20^{\circ} \mathrm{C}\right.\right.$, calculated-density) 155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
89.0 ( $m$ - and $p$-methylstyrene commercial product, Dreisbach 1955) 89.0, 100 (quoted, $m$ - and $p$-methylstyrene, calculated-group contribution, Irmann 1965)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
2693* $\quad\left(67.6^{\circ} \mathrm{C}\right.$, mercury manometer, measured range $67.6-169.1^{\circ} \mathrm{C}$, Buck et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=-3563 /(\mathrm{T} / \mathrm{K})-7.553 \cdot \log (\mathrm{~T} / \mathrm{K})+30.90$; temp range $80-120^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
687* (41.48 ${ }^{\circ} \mathrm{C}$, differential manometer, Clements et al. 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=6.95079-1520.412 /\left(210.967+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $41.48-111.8^{\circ} \mathrm{C}$ (Antoine eq. from differential manometer measurements, measured range $41.48-111.8^{\circ} \mathrm{C}$, Clements et al. 1953)
257 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.99468-1553.4 /\left(206.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-225^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)

228, 244 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.06423-1564.74 /\left(204.083+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $67.6-169^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.11224-1615.091 /\left(210.809+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $41.7-111.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{atm})=(1-442.985 / \mathrm{T}) \times 10^{\wedge}\left(0.885861-7.19653 \times 10^{4} \cdot \mathrm{~T}+6.75359 \times 10^{7} \cdot \mathrm{~T}^{2}\right) ; \mathrm{T}$ in K , temp range 314.93-442.15 K (Cox vapor pressure eq., Chao et al. 1983)

227, 244 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.17253-1553.744 /\left(202.922+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $67.6-169.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.22823-1609.825 /\left(210.331+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $41.7-111.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.27534-1695.4 /\left(220.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $10-72^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.87928-1471.28 /\left(200.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $72-250^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)

245 (Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.07569-1520.412 /(-71.183+\mathrm{T} / \mathrm{K})$; temp range $314-385 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=11.6959-2.9912 \times 10^{3} /(\mathrm{T} / \mathrm{K})+0.33334 \cdot \log (\mathrm{~T} / \mathrm{K})-8.8935 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+4.9793 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $187-657 \mathrm{~K}$ (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
387 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
3.35 (Leo et al. 1971)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
1.50 (gold fish, flow-through method, Ogata et al. 1984)
1.50, 1.63 (gold fish, quoted, calculated-MCI $\chi$, Ogata et al. 1984)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.39.1
Reported vapor pressures of $m$-methylstyrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

Buck et al. 1949

| Hg manometer |  |  |  | differential manometer |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 67.6 | 2693 | eq. $4 \mathrm{t} /{ }^{\circ} \mathrm{C}$ | P/mmHg | 41.48 | 687 | 99.33 | 10696 |
| 72.3 | 3440 | A | 30.9 | 43.22 | 744 | 111.8 | 17020 |
| 80.7 | 4933 | B | 3563 | 49.49 | 1104 |  |  |
| 87 | 6533 | C | 7.553 | 52.12 | 1261 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -86.34 |
| 93.8 | 8373 |  |  | 55.73 | 1499 | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 171.6 |
| 96.6 | 9733 |  |  | 57.8 | 1673 |  |  |
| 106.9 | 14399 |  |  | 65.2 | 2445 | $\Delta \mathrm{H}_{\mathrm{V}}=38.7$ | $\mathrm{J} / \mathrm{mol}$ |
| 121 | 12998 |  |  | 70.95 | 3192 |  |  |
| 128.3 | 30398 |  |  | 71.01 | 3202 | eq. 2 | mmHg |
| 138.5 | 41597 |  |  | 71.02 | 3204 | A | 6.95079 |
| 147.6 | 54795 |  |  | 71.1 | 3248 | B | 1520.412 |
| 159.2 | 75727 |  |  | 77.12 | 4234 | C | 201.967 |
| 169.1 | 98392 |  |  |  |  |  |  |



FIGURE 3.1.1.39.1 Logarithm of vapor pressure versus reciprocal temperature for m-methylstyrene.

### 3.1.1.40 p-Methylstyrene



Common Name: $p$-Methylstyrene
Synonym: methylvinylbenzene, 4-vinyl toluene, $p$-methylvinylbenzene
Chemical Name: 4-methylstyrene
CAS Registry No: 622-97-9
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{10}, 4-\mathrm{CH}_{3} \mathrm{C}_{6} \mathrm{H}_{4} \mathrm{CH}=\mathrm{CH}_{2}$
Molecular Weight: 118.17
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -34.1 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 172.8 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.9016,0.9060 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
$0.8760 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$129.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 155.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
89.0 (quoted, $m$ - and $p$-methylstyrene commercial product, Dreisbach 1955)
89.0, 100 (quoted, $m$ - and $p$-methylstyrene, calculated-group contribution, Irmann 1965)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* $\quad\left(16^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $16-175^{\circ} \mathrm{C}$, Stull 1947)

2773* ( $68.6^{\circ} \mathrm{C}$, mercury manometer, measured range $68.6-170^{\circ} \mathrm{C}$, Buck et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=-3476 /(\mathrm{T} / \mathrm{K})-6.923 \cdot \log (\mathrm{~T} / \mathrm{K})+29.03$; temp range $80-120^{\circ} \mathrm{C}$ (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=7.34046-1791.0 /\left(230+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ (Antoine eq., Dreisbach \& Martin 1949)
4954* $\quad\left(90.98^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $90.98-171.06^{\circ} \mathrm{C}$, Dreisbach \& Shrader 1949)
$376^{*} \quad\left(31.82^{\circ} \mathrm{C}\right.$, differential manometer, measured range $31.8-96.9^{\circ} \mathrm{C}$, Clements et al. 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0483-1594.747 /\left(209.889+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $31.8-96.9^{\circ} \mathrm{C}$ (Antoine eq. from differential manometer measurements, Clements et al. 1953)
241.5 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.35420-1765.6 /\left(223.8+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $75-205^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 10724.2 /(\mathrm{T} / \mathrm{K})]+8.130903$; temp range $16.0-175^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ ) 216.6, 241 (extrapolated-Antoine eq., Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01119-1535.073 /\left(200.732+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $68.6-170^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{mmHg})=6.11531-1591.082 /\left(209.441+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $31.8-96.93^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)
$\log (\mathrm{P} / \mathrm{atm})=\left(1-443.748 /(\mathrm{T} / \mathrm{K}) \times 10^{\wedge}\left[0.875061-7.08160 \times 10^{4} \cdot(\mathrm{~T} / \mathrm{K})+7.33467 \times 10^{7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right] ;\right.$ temp range: $289.15-443.15 \mathrm{~K}$, (Cox vapor pressure eq., Chao et al. 1983)
215, 241 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.11531-1521.514 /\left(199.299+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $68.6-170^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.16144-1586.596 /\left(209.046+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $31.8-96.93^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0112-1535.1 /\left(200.7+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $68-170^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
242 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1732-1594.147 /(-63.261+\mathrm{T} / \mathrm{K})$; temp range $304-370 \mathrm{~K}$ (liquid, Antoine eq., Stephenson $\&$ Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=50.6506-4.0628 \times 10^{3} /(\mathrm{T} / \mathrm{K})-15.524 \cdot \log (\mathrm{~T} / \mathrm{K})+5.5381 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-1.1313 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2}$, temp range 239-665 K (Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
287 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.35 (Leo et al. 1971; quoted, Ogata et al. 1984)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
1.55 (gold fish, flow-through method, Ogata et al. 1984)
$1.55,1.62$ (gold fish, quoted, calculated-MCI $\chi$, Ogata et al. 1984)
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 3.1.1.40.1
Reported vapor pressures of pmethylstyrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$

| Stull 1947 |  | Buck et al. 1949 |  | Dreisbach \& Shrader 1949 |  | Clements et al. 1953 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | Hg manometer |  | ebulliometry |  | differential manometer |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 16 | 133.3 | 68.6 | 2773 | 90.98 | 4954 | 31.82 | 376 |
| 42 | 666.6 | 70.6 | 2986 | 98.13 | 10351 | 41.76 | 689 |
| 55.1 | 1333 | 75.1 | 3733 | 116.06 | 16959 | 41.83 | 693 |
| 6.2 | 2666 | 78.8 | 4400 | 171.06 | 101325 | 52.17 | 1207 |
| 85 | 5333 | 80.6 | 4720 |  |  | 53.94 | 1331 |
| 95 | 7999 | 82.7 | 5200 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -70.3 | 59.56 | 1797 |
| 108.6 | 13332 | 84.2 | 5573 | bp/ ${ }^{\circ} \mathrm{C}$ | 171.06 | 59.91 | 1855 |
| 128.7 | 26664 | 87 | 6559 |  |  | 66.62 | 2538 |
| 151.2 | 53329 | 94.1 | 8559 |  |  | 75.4 | 3858 |
| 175 | 101325 | 104.4 | 12826 |  |  | 76.19 | 3974 |
|  |  | 115.1 | 18958 |  |  | 80.2 | 4718 |

TABLE 3.1.1.40.1 (Continued)

| Stull 1947 |  | Buck et al. 1949 |  | Dreisbach \& Shrader 1949 |  | Clements et al. 1953 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | Hg manometer |  | ebulliometry |  | differential manometer |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| mp/ ${ }^{\circ} \mathrm{C}$ | - | 131.9 | 33197 |  |  | 82.44 | 5208 |
|  |  | 144 | 47996 |  |  | 90.9 | 7439 |
|  |  | 154.7 | 65728 |  |  | 96.93 | 9466 |
|  |  | 163.7 | 83193 |  |  |  |  |
|  |  | 170 | 99725 |  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -34.15 |
|  |  |  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 172.78 |
|  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -37.8 |  |  | $\Delta \mathrm{H}_{\mathrm{V}}$ | $95 \mathrm{~kJ} / \mathrm{mol}$ |
|  |  | $\text { eq. } 4$ | $\mathrm{P} / \mathrm{mmHg}$ |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | A | 29.03 |  |  | A | 7.0483 |
|  |  | B | 3476 |  |  | B | 1594.747 |
|  |  | C | 6.923 |  |  | C | 209.889 |



FIGURE 3.1.1.40.1 Logarithm of vapor pressure versus reciprocal temperature for $p$-methylstyrene.

### 3.1.1.41 Tetralin



Common Name: Tetralin
Synonym: naphthalene-1,2,3,4-tetrahydride
Chemical Name: 1,2,3,4-tetrahydronaphthalene
CAS Registry No: 119-64-2
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{12}$
Molecular Weight: 132.202
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-35.7 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
207.6 (Weast 1982-83; Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.9702
$\left(20^{\circ} \mathrm{C}\right.$, Weast $1982-83$; Dean 1985)
$0.9695,0.9660 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$136.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated- density)
177.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
12.477 (Riddick et al. 1986)
12.45 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
52.44, 49.6 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
14.94 (calculated-QSAR Data base, Passino \& Smith 1987)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2666* ( $93.8^{\circ} \mathrm{C}$, temp range $93.8-171.06^{\circ} \mathrm{C}$, Herz \& Schuftan 1922)
53.3* (mercury manometer, measured range $-2.4-65^{\circ} \mathrm{C}$, Linder 1931)
$66.66^{*} \quad\left(39.3^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $39.3-148.6^{\circ} \mathrm{C}$, Gardner \& Brewer 1937)
$133.3^{*} \quad\left(38^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $38-207^{\circ} \mathrm{C}$, Stull 1947)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 11613.0 /(\mathrm{T} / \mathrm{K})]+8.194951$; temp range $38-207.2^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$1737 * \quad\left(82.3^{\circ} \mathrm{C}\right.$, diaphragm gauge, measured range $82.3-276.21^{\circ} \mathrm{C}$, Nasir et al. 1980)
$\log (\mathrm{P} / \mathrm{mmHg})=[1-480.364 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.85916-5.75417 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+4.41971 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $311.15-710.93 \mathrm{~K}$, (Cox eq., Chao et al. 1983)
53.75 (extrapolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.07055-1741.30 /\left(208.26+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $94-206^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
53.0 (selected lit. average, Riddick et al. 1986)
$\log (\mathrm{P} / \mathrm{kPa})=11.079-2797.90 /(\mathrm{T} / \mathrm{K})+1.187 \cdot \log (\mathrm{~T} / \mathrm{K})$, temp range not specified (Antoine eq., Riddick et al. 1986)
56.7 (Antoine eq., extrapolated, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.35719-1854.82 /(-54.237+\mathrm{T} / \mathrm{K})$; temp range $311-481 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=39.9174-4.132 \times 10^{3} /(\mathrm{T} / \mathrm{K})-10.78 \cdot \log (\mathrm{~T} / \mathrm{K})+1.9691 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+2.0405 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2}$, temp range $237-720 \mathrm{~K}$ (Yaws 1994)
$38.35^{*} \quad\left(20.26^{\circ} \mathrm{C}\right.$, static method, measured range 253.8-442.8 K, Mokbel et al. 1998)

Henry's Law Constant $\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right.$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$76.0,106.4,137.8,189.5,271.6 \quad\left(0,15,20,25.30^{\circ} \mathrm{C}\right.$, EPICS-GC, Ashworth et al. 1988)
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \mathrm{m} \mathrm{mol}^{-1}\right)\right]=11.83-5392 /(\mathrm{T} / \mathrm{K})$; temp range $10-30^{\circ} \mathrm{C}$ (EPICS-GC, Ashworth et al. 1988)
$142.8 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from literature experimentally measured data, Staudinger \& Roberts 1996 , 2001) $\log \mathrm{K}_{\mathrm{AW}}=6.332-2215 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
3.83 (calculated-fragment const., Rekker 1977)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k , and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO} 3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{03}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(3.43 \pm 0.06) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{NO} 3}=(8.6 \pm 1.3) \times 10^{-15} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at room temp. (relative rate method, Atkinson \& Aschmann 1988)
$\mathrm{k}_{\mathrm{OH}}=3.43 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=11.4 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ exptl $)=34.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (SAR [structure-activity relationship], Kwok \& Atkinson 1995)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
Half-Lives in the Environment:

TABLE 3.1.1.41.1
Reported vapor pressures of tetralin at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| Herz \& Schuftan 1922 |  | Stull 1947 |  | Gardner \& Brewer 1937 |  | Mokbel et al. 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | summary of literature data |  | ebulliometry |  | static method |  |
|  |  | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| 93.8 | 2666 | 38 | 133 | 39.3 | 66.66 | 253.8 | 1.279 |
| 103 | 4000 | 65.3 | 666.6 | 40.1 | 79.99 | 264.01 | 3.349 |
| 140 | 15732 | 79 | 1333 | 40.8 | 93.33 | 273.65 | 7.984 |
| 150 | 21598 | 93.8 | 2666 | 41.8 | 93.33 | 283.54 | 17.94 |
| 167.5 | 36397 | 110 | 5333 | 46.6 | 226.7 | 293.51 | 38.35 |
| 206.2 | 98658 | 121.3 | 7999 | 48.9 | 253.3 | 303.52 | 78.52 |
|  |  | 135.3 | 13332 | 49.4 | 253.3 | 313.51 | 153.0 |
|  |  | 157.2 | 26664 | 54 | 293.3 | 323.55 | 284.0 |
|  | Linder 1931 | 181.8 | 53329 | 74.4 | 946.6 | 333.57 | 506.0 |
| mercury manometer |  | 207.2 | 101325 | 75.1 | 959.9 | 343.62 | 868.0 |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -31.0 | 101.1 | 3040 | 353.66 | 1443 |
|  |  |  |  | 126.6 | 9040 | 358.64 | 1801 |
| -2.4 | 2 |  |  | 148.6 | 19625 | 363.62 | 2254 |
| -1.2 | 3.133 |  |  |  |  | 373.66 | 3508 |
| 25 | 53.33 |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 210.5 | 383.00 | 5179 |
| 65 | 110.7 |  |  |  |  | 392.95 | 7617 |
|  |  |  |  |  |  | 402.89 | 10948 |
|  |  |  |  | Nasir et al. 1980 |  | 412.86 | 15444 |
|  |  |  |  | diaphragm gauge |  | 422.82 | 21388 |
|  |  |  |  | t/ ${ }^{\circ} \mathbf{C}$ | P/Pa | 432.84 | 29254 |
|  |  |  |  |  |  | 442.80 | 39128 |
|  |  |  |  | 82.3 | 1737 |  |  |
|  |  |  |  | 125.81 | 10500 | data fit | Wagner eq. |
|  |  |  |  | 150.15 | 22419 |  |  |
|  |  |  |  | 200.11 | $84002$ |  |  |
|  |  |  |  | 250.66 | 257307 |  |  |
|  |  |  |  | 276.21 | 348091 |  |  |



FIGURE 3.1.1.41.1 Logarithm of vapor pressure versus reciprocal temperature for tetralin.

TABLE 3.2.1
Summary of the physical properties of mononuclear aromatic hydrocarbons

| Compound | CAS no. | Molecular formula | Molecular weight, MW $\mathrm{g} / \mathrm{mol}$ | $\underset{{ }^{\circ} \mathrm{C}}{\substack{ \\\hline}}$ | $\begin{aligned} & \text { bp } \\ & { }^{\circ} \mathrm{C} \end{aligned}$ | Fugacity ratio, F at $25{ }^{\circ} \mathbf{C}^{*}$ | Density, $\rho \mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ | Molar volume, $\mathrm{V}_{\mathrm{M}}$ $\mathrm{cm}^{3} / \mathrm{mol}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  | MW/p <br> at $20^{\circ} \mathrm{C}$ | Le Bas |
| Benzene | 71-43-2 | $\mathrm{C}_{6} \mathrm{H}_{6}$ | 78.112 | 5.49 | 80.09 | 1 | 0.8765 | 89.12 | 96.0 |
| Toluene | 108-88-3 | $\mathrm{C}_{7} \mathrm{H}_{8}$ | 92.139 | -94.95 | 110.63 | 1 | 0.8668 | 106.30 | 118.2 |
| Ethylbenzene | 100-41-4 | $\mathrm{C}_{8} \mathrm{H}_{10}$ | 106.165 | -94.96 | 136.19 | 1 | 0.867 | 122.45 | 140.4 |
| $o$-Xylene | 95-47-6 | $\mathrm{C}_{8} \mathrm{H}_{10}$ | 106.165 | -25.2 | 144.5 | 1 | 0.8802 | 120.61 | 140.4 |
| $m$-Xylene | 108-38-3 | $\mathrm{C}_{8} \mathrm{H}_{10}$ | 106.165 | -47.8 | 139.12 | 1 | 0.8842 | 120.07 | 140.4 |
| $p$-Xylene | 106-42-3 | $\mathrm{C}_{8} \mathrm{H}_{10}$ | 106.165 | 13.25 | 138.37 | 1 | 0.8611 | 123.29 | 140.4 |
| 1,2,3-Trimethylbenzene | 526-73-8 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -25.4 | 176.12 | 1 | 0.8944 | 134.38 | 162.6 |
| 1,2,4-Trimethylbenzene | 95-63-6 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -43.77 | 169.38 | 1 | 0.8758 | 137.24 | 162.6 |
| 1,3,5-Trimethylbenzene | 108-67-8 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -44.72 | 164.74 | 1 | 0.8800 | 136.58 | 162.6 |
| $n$-Propylbenzene | 103-65-1 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -99.6 | 159.24 | 1 | 0.862 | 139.43 | 162.6 |
| Isopropylbenzene | 98-82-8 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -96.02 | 152.41 | 1 | 0.8618 | 139.47 | 162.6 |
| 1-Ethyl-2-methylbenze ne ( $o$-Ethyltoluene) | 611-14-3 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -79.83 | 165.2 | 1 | 0.8807 | 136.47 | 162.6 |
| 1-Ethyl-3-methylbenze ne ( $m$-Ethyltoluene) | 620-14-4 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -95.6 | 161.3 | 1 | 0.8645 | 139.03 | 162.6 |
| 1-Ethyl-4-methylbenze ne ( $p$-Ethyltoluene) | 622-96-8 | $\mathrm{C}_{9} \mathrm{H}_{12}$ | 120.191 | -62.35 | 162 | 1 | 0.8614 | 139.53 | 162.6 |
| Isopropyl-4-methylben zene ( $p$-Cymene) | 99-87-6 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -67.94 | 177.1 | 1 | 0.8573 | 156.56 | 184.8 |
| $n$-Butylbenzene | 104-51-8 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -87.85 | 183.31 | 1 | 0.8601 | 156.05 | 184.8 |
| Isobutylbenzene | 538-93-2 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -51.4 | 172.79 | 1 | 0.8532 | 157.31 | 184.8 |
| sec-Butylbenzene | 135-98-8 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -82.7 | 173.3 | 1 | 0.8621 | 155.69 | 184.4 |
| tert-Butylbenzene | 98-06-6 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -57.8 | 169.1 | 1 | 0.8665 | 154.90 | 184.8 |
| 1,2,3,4-Tetramethylben zene | 488-23-3 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -6.2 | 205 | 1 | 0.9052 | 148.27 | 184.8 |
| 1,2,3,5-Tetramethylben zene | 527-53-7 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | -23.7 | 198 | 1 | 0.8903 | 150.76 | 184.8 |
| 1,2,4,5-Tetramethylben zene | 95-93-2 | $\mathrm{C}_{10} \mathrm{H}_{14}$ | 134.218 | 79.3 | 196.8 | 0.293 | 0.8380 | 160.16 | 184.8 |
| $n$-Pentylbenzene | 538-68-1 | $\mathrm{C}_{11} \mathrm{H}_{16}$ | 148.245 | -75 | 205.4 | 1 | 0.8585 | 172.68 | 207.0 |


| Pentamethylbenzene | $700-12-9$ | $\mathrm{C}_{11} \mathrm{H}_{16}$ | 148.245 | 54.5 | 232 | 0.514 | 0.917 | 161.66 | 207.0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $n$-Hexylbenzene | $1077-16-3$ | $\mathrm{C}_{12} \mathrm{H}_{18}$ | 162.271 | -61 | 226.1 | 1 | 0.8613 | 188.40 | 229.2 |
| Hexamethylbenzene | $87-85-4$ | $\mathrm{C}_{12} \mathrm{H}_{18}$ | 162.271 | 165.5 | 263.4 | 0.0418 | 1.063 | $152.65 \#$ | 229.2 |
| Heptylbenzene | $1078-71-3$ | $\mathrm{C}_{13} \mathrm{H}_{20}$ | 176.298 | -48 | 240 | 1 | 0.8567 | 205.79 | 251.4 |
| Octylbenzene | $2189-60-8$ | $\mathrm{C}_{14} \mathrm{H}_{22}$ | 190.325 | -36 | 264 | 1 | 0.8562 | 222.29 | 273.6 |
| Nonylbenzene | $1081-77-2$ | $\mathrm{C}_{15} \mathrm{H}_{24}$ | 204.352 | -24 | 280.5 | 1 | 0.8584 | 238.06 | 295.8 |
| Decylbenzene | $104-72-3$ | $\mathrm{C}_{16} \mathrm{H}_{26}$ | 218.377 | -14.4 | 293 | 1 | 0.8555 | 255.26 | 318.0 |
| Undecylbenzene | $6742-54-7$ | $\mathrm{C}_{17} \mathrm{H}_{28}$ | 232.404 | -5 | 316 | 1 | 0.8553 | 271.72 | 340.2 |
| Dodecylbenzene | $123-01-3$ | $\mathrm{C}_{18} \mathrm{H}_{30}$ | 246.431 | 3 | 328 | 1 | 0.8551 | 288.19 | 362.4 |
| Tridecylbenzene | $123-02-4$ | $\mathrm{C}_{19} \mathrm{H}_{32}$ | 260.457 | 10 | 346 | 1 | 0.8550 | 304.63 | 384.6 |
| Tetradecylbenzene | $1459-10-5$ | $\mathrm{C}_{20} \mathrm{H}_{34}$ | 274.484 | 16 | 359 | 1 | 0.8549 | 321.07 | 406.8 |
| Styrene | $100-42-5$ | $\mathrm{C}_{8} \mathrm{H}_{8}$ | 104.150 | -30.65 | 145 | 1 | 0.9060 | 114.96 | 133.0 |
| $o$-Methylstyrene | $611-15-4$ | $\mathrm{C}_{9} \mathrm{H}_{10}$ | 118.175 | -68.5 | 169.8 | 1 | 0.9106 | 129.78 | 155.2 |
| $m$-Methylstyrene | $100-80-1$ | $\mathrm{C}_{9} \mathrm{H}_{10}$ | 118.175 | -86.3 | 164 | 1 | 0.9028 | 130.90 | 155.2 |
| $p$-Methylstyrene | $622-97-9$ | $\mathrm{C}_{9} \mathrm{H}_{10}$ | 118.175 | -34.1 | 172.8 | 1 | 0.9016 | 131.07 | 155.2 |
| $\alpha$-Methylstyrene | $98-83-9$ | $\mathrm{C}_{9} \mathrm{H}_{10}$ | 118.175 | -23.2 | 165.4 | 1 | 0.9106 | 129.78 | 155.2 |
| $\beta$-Methylstyrene, cis- | $766-90-5$ | $\mathrm{C}_{9} \mathrm{H}_{10}$ | 118.175 | -61.6 | 167.5 | 1 | 0.9088 | 130.03 | 155.2 |
| $\beta$-Methylstyrene, trans- | $873-66-5$ | $\mathrm{C}_{9} \mathrm{H}_{10}$ | 118.175 | -29.3 | 178.3 | 1 | 0.9023 | $130.97 \#$ | 155.2 |
| Tetralin | $119-64-2$ | $\mathrm{C}_{10} \mathrm{H}_{12}$ | 132.202 | -35.7 | 207.6 | 1 | 0.9695 | 136.36 | 177.4 |

* Assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$.
\# at $25^{\circ} \mathrm{C}$.

TABLE 3.2.2
Summary of selected physical-chemical properties of mononuclear aromatic hydrocarbons at $25^{\circ} \mathrm{C}$

| Compound | Selected properties: |  |  |  |  |  | Henry's law constant |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Vapor pressure |  | Aqueous solubility |  |  |  |  |
|  | Ps/Pa | $\mathbf{P}_{\mathbf{L}} / \mathbf{P a}$ | $\mathbf{S} /\left(\mathrm{g} / \mathrm{m}^{3}\right)$ | $\begin{gathered} \mathrm{C}^{\mathrm{S}} /(\mathrm{mol} / \\ \left.\mathrm{m}^{3}\right) \end{gathered}$ | $\begin{gathered} \mathrm{C}_{\mathrm{L}} /(\mathrm{mol} / \\ \left.\mathrm{m}^{3}\right) \end{gathered}$ | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {Ow }}$ | $\mathrm{H} /\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)$ calculated P/C |
| Benzene | 12700 | 12700 | 1780 | 22.788 | 22.788 | 2.13 | 557 |
| Toluene | 3800 | 3800 | 515 | 5.590 | 5.590 | 2.69 | 680 |
| Ethylbenzene | 1270 | 1270 | 152 | 1.431 | 1.431 | 3.13 | 887 |
| $o$-Xylene | 1170 | 1170 | 220 | 2.072 | 2.072 | 3.15 | 565 |
| $m$-Xylene | 1100 | 1100 | 160 | 1.507 | 1.507 | 3.20 | 730 |
| p-Xylene | 1170 | 1170 | 215 | 2.024 | 2.024 | 3.18 | 578 |
| 1,2,3-Trimethylbenzene | 200 | 200 | 70 | 0.582 | 0.582 | 3.55 | 343 |
| 1,2,4-Trimethylbenzene | 270 | 270 | 57 | 0.474 | 0.474 | 3.60 | 569 |
| 1,3,5-Trimethylbenzene | 325 | 325 | 50 | 0.416 | 0.416 | 3.58 | 781 |
| $n$-Propylbenzene | 450 | 450 | 52 | 0.433 | 0.433 | 3.69 | 1040 |
| Isopropylbenzene | 610 | 610 | 50 | 0.416 | 0.416 | 3.63 | 1466 |
| 1-Ethyl-2-methylbenzene | 330 | 330 | 75 | 0.624 | 0.624 | 3.63 | 529 |
| 1-Ethyl-3-methylbenzene | 391 | 391 |  |  |  |  |  |
| 1-Ethyl-4-methylbenzene | 395 | 395 | 95 | 0.790 | 0.790 | 3.63 | 500 |
| Isopropyl-4-methylbenzene | 204 | 204 | 34 | 0.253 | 0.253 | 4.10 | 805 |
| $n$-Butylbenzene | 137 | 137 | 13.8 | 0.103 | 0.103 | 4.26 | 1332 |
| Isobutylbenzene | 250 | 250 | 10.1 | 0.075 | 0.075 | 4.01 | 3322 |
| sec -Butylbenzene | 240 | 240 | 17 | 0.127 | 0.127 |  | 1890 |
| tert-Butylbenzene | 286 | 286 | 30 | 0.224 | 0.224 | 4.11 | 1280 |
| 1,2,3,4-Tetramethylbenzene | 45 | 45 |  |  |  | 3.90 |  |
| 1,2,3,5-Tetramethylbenzene | 62 | 62 |  |  |  | 4.04 |  |
| 1,2,4,5-Tetramethylbenzene | 66 | 66 | 3.48 | 0.026 | 0.026 | 4.10 | 2546 |
| $n$-Pentylbenzene | 44 | 44 | 3.85 | 0.026 | 0.026 | 4.90 | 1694 |
| Pentamethylbenzene | 9.52 | 18.63 | 15.5 | 0.105 | 0.205 |  |  |
| $n$-Hexylbenzene | 13.61 | 13.61 | 1.02 | 0.006 | 0.006 | 5.52 | 2165 |
| Hexamethylbenzene | 0.155 | 3.90 | 0.235 | 0.001 | 0.036 | 4.61 |  |
| Heptylbenzene | 3.95 | 3.95 |  |  |  | 5.37 |  |
| Octylbenzene | 2.03 | 2.03 |  |  |  | 6.30 |  |
| Nonylbenzene | 0.30 | 0.30 |  |  |  | 6.82 |  |
| Decylbenzene | 0.077 | 0.077 |  |  |  | 7.37 |  |


| Undecylbenzene | 0.045 | 0.045 |  | 8.14 |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Dodecylbenzene | 0.017 | 0.017 |  | 8.65 |  |
| Tridecylbenzene | 0.00070 | 0.0007 |  | 9.36 |  |
| Tetradecylbenzene | 0.000113 | 0.000113 |  | 9.95 |  |
| Styrene | 880 | 880 | 250 | 2.40 | 2.40 |
| $o$-Methylstyrene | 245 | 245 |  |  |  |
| $m$-Methylstyrene | 250 | 250 |  | 3.35 |  |
| $p$-Methylstyrene | 242 | 242 |  | 3.35 |  |
| $\alpha$-Methylstyrene | 324 | 324 | 3.48 |  |  |
| $\beta$-Methylstyrene, cis- | 258 | 258 | 3.35 |  |  |
| $\beta$-Methylstyrene, trans- | 216.6 | 216.6 |  |  |  |
| Tetralin | 54 | 54 | 3.83 |  |  |

TABLE 3.2.3
Suggested half-life classes of mononuclear aromatic hydrocarbons in various environmental compartments at $25^{\circ} \mathrm{C}$

| Compound | Air <br> class | Water <br> class | Soil <br> class | Sediment <br> class |
| :--- | :---: | :---: | :---: | :---: |
| Benzene | 3 | 4 | 5 | 6 |
| Toluene | 2 | 5 | 6 | 7 |
| Ethyl benzene | 2 | 5 | 6 | 7 |
| $o$-Xylene | 2 | 5 | 6 | 7 |
| $m$-Xylene | 2 | 5 | 6 | 7 |
| $p$-Xylene | 2 | 5 | 7 |  |
| 1,2,3-Trimethylbenzene | 2 | 5 | 6 | 7 |
| 1,2,4-Trimethylbenzene | 2 | 5 | 7 |  |
| 1,3,5-Trimethylbenzene | 2 | 5 | 6 | 7 |
| $n$-Propylbenzene | 2 | 5 | 6 | 7 |
| Isopropylbenzene | 2 | 5 | 6 | 7 |
| 1-Isopropyl-4-methylbenzene $(p-C y m e n e)$ | 2 | 5 | 6 | 7 |
| 1,2,4,5-Tetramethylbenzene | 2 | 5 |  | 7 |

where,

| Class | Mean half-life <br> (hours) | Range (hours) |
| :--- | :--- | :--- |
| 1 | 5 | $<10$ |
| 2 | $17(\sim 1$ day $)$ | $10-30$ |
| 3 | $55(\sim 2$ days $)$ | $30-100$ |
| 4 | $170(\sim 1$ week $)$ | $100-300$ |
| 5 | $550(\sim 3$ weeks $)$ | $300-1,000$ |
| 6 | $1700(\sim 2$ months $)$ | $1,000-3,000$ |
| 7 | $5500(\sim 8$ months $)$ | $3,000-10,000$ |
| 8 | $17000(\sim 2$ years $)$ | $10,000-30,000$ |
| 9 | $55000(\sim 6$ years $)$ | $>30,000$ |



FIGURE 3.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 3.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 3.2.3 Octanol-water partition coefficient versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 3.2.4 Henry's law constant versus Le Bas molar volume for mononuclear aromatic hydrocarbons.


FIGURE 3.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for mononuclear aromatic hydrocarbons.

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### 4.1. LIST OF CHEMICALS AND DATA COMPILATIONS

### 4.1.1 Polynuclear aromatic hydrocarbons (PAHs)

### 4.1.1.1. Indan



Common Name: Indan
Synonym: hydroindene, 2,3-dihydroindene, 2,3-dihydro-1H-indene, indane
Chemical Name: indan
CAS Registry No: 496-11-7
Molecular Formula: $\mathrm{C}_{9} \mathrm{H}_{10}$
Molecular Weight: 118.175
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): -51.38 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 177.97 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ : 0.9639 (Weast 1982-83; Dean 1985; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): $123.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density) 143.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $49 \pm 1.5 \quad$ (Ambrose \& Sprake 1976)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 8.60 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
38.77, 45.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
88.9 (shake flask-GC, Price 1976)
109.1 (shake flask-fluorescence, Mackay \& Shiu 1977)

100 (recommended-IUPAC, Shaw 1989)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated ${ }^{*}$, are compiled at the end of this section):
5523* $\quad\left(91.68^{\circ} \mathrm{C}\right.$, ebulliometry, measured range $91.68-129.05^{\circ} \mathrm{C}$, Stull et al. 1961)
204.0* (comparative ebulliometry, extrapolated from vapor pressure equation derived from exptl data, Ambrose \& Sprake 1976)
$\log (\mathrm{P} / \mathrm{kPa})=6.10462-1574.160 /[(\mathrm{T} / \mathrm{K})-67.079$; temp range $355.006-482.437 \mathrm{~K}$ (vapor pressure eq., ebulliometry, Ambrose \& Sprake 1976)
$9585^{*} \quad\left(101.124^{\circ} \mathrm{C}\right.$, comparative ebulliometry, measured range $101.124-192.408^{\circ} \mathrm{C}$, Osborn \& Scott 1978) $\log (\mathrm{P} / \mathrm{atm})=[1-451.051 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.859420-6.08324 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+4.77502 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; temp range 355.01-452.24 K (Cox eq., Chao et al. 1983)
195.6 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.1012-1571.723 /\left(205.798+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $81.86-209.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Ambrose \& Sprake 1976, Boublik et al. 1984)
196.9 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.11622-1580.315 /(-66.49+\mathrm{T} / \mathrm{K})$; temp range $374-466 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.33 (Hansch \& Leo 1979)
3.30 (calculated-TSA, Yalkowsky \& Valvani 1976)
3.57 (calculated-fragment const., Valvani \& Yalkowsky 1980)
3.29 (calculated-solubility, Mackay et al. 1980)
3.31 (calculated-fragment const., Yalkowsky et al. 1983)
3.33 (shake flask, Log P Database, Hansch \& Leo 1987)
3.36 (calculated-molar volume, Wang et al. 1991)
3.33 (recommended, Sangster 1993)
3.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: photolysis rate $\mathrm{k}<3 \times 10^{-5} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}>1 \mathrm{~d}$ (Kwok et al. 1997)
Oxidation: rate constant k for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated; $*$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=9.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}(\operatorname{exptl})=(19 \pm 5) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=8.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated
lifetime of $8 \mathrm{~h} ; \mathrm{k}_{\mathrm{NO}_{3}}(\operatorname{exptl})=(6.6 \pm 2.0) \times 10^{-15} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated lifetime of 7 d ; and $\mathrm{k}_{\mathrm{O}_{3}}($ exptl $)<3 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated lifetime of $>55 \mathrm{~d}$ at $297 \pm 2 \mathrm{~K}$ (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: photolysis $\mathrm{t}_{1 / 2}>1 \mathrm{~d}$; calculated tropospheric lifetimes of $8 \mathrm{~h}, 7 \mathrm{~d}$ and $>55 \mathrm{~d}$ due to reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$, respectively, at room temp. (Kwok et al. 1997)

## TABLE 4.1.1.1.1

Reported vapor pressures of indan at various temperatures and the coefficients for the vapor pressure equations

```
log P = A - B/(T/K)
log P = A - B/(C+t/ }\mp@subsup{}{}{\circ}\textrm{C}
log P = A - B/(C + T/K)
log P = A - B/(T/K) - C log (T/K)
```

$$
\begin{align*}
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) \tag{2}
\end{align*}
$$

Stull et al. 1961 Ambrose \& Sprake 1976

| ebulliometry |  | comparative ebulliometry |  | comparative ebulliometry |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 91.68 | 5523 | 81.856 | 4343 | 101.124 | 9585 |
| 107.38 | 12086 | 88.012 | 5650 | 104.381 | 10887 |
| 128.56 | 25246 | 93.482 | 7069 | 107.849 | 12339 |
| 152.36 | 51766 | 98.033 | 6471 | 111.229 | 13955 |
| 176.03 | 96999 | 101.96 | 9860 | 114.621 | 15748 |

(Continued)

TABLE 4.1.1.1.1 (Continued)

| Stull et al. 1961 |  | Ambrose \& Sprake 1976 |  | Osborn \& Scott 1978 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | comparative ebulliometry |  | comparative ebulliometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 178.04 | 101729 | 109.194 | 12920 | 118.027 | 17735 |
| 129.05 | 104442 | 116.391 | 16722 | 121.442 | 19933 |
|  |  | 120.345 | 19150 | 128.315 | 25023 |
| $\mathrm{mp} / \mathrm{K}$ | 221.77 | 123.556 | 21300 | 135.235 | 31177 |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=8.60$ |  | 128.597 | 25174 | 142.204 | 38565 |
| Antoine eq. |  | 134.718 | 30586 | 149.224 | 47375 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 139.494 | 35453 | 156.300 | 57817 |
| A | 7.05483 | 146.528 | 43667 | 263.418 | 70120 |
| B | 1625.70 | 152.479 | 51799 | 170.590 | 84432 |
| C | 211.645 | 158.969 | 61998 | 177.812 | 101325 |
|  |  | 164.763 | 72392 | 177.812 | 101325 |
|  |  | 171.453 | 86085 | 177.811 | 101325 |
|  |  | 176.521 | 97757 | 185.085 | 120790 |
|  |  | 177.075 | 99114 | 192.408 | 143240 |
|  |  | 177.531 | 100222 |  |  |
|  |  | 25.0 | 204.0 | $\Delta \mathrm{H}_{\mathrm{v}} /$ | $39.67$ |
|  |  | bp/K | $451.12 \mathrm{~K}$ | $\Delta \mathrm{H}_{\mathrm{V}} /$ | $49.03$ |
|  |  | $\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{k}$ $\Delta \mathrm{H}_{\mathrm{V}}$ | $\begin{aligned} & 39.8 \text { at bp } \\ & =49.0 \\ & \text { at } 298.15 \mathrm{~K} \end{aligned}$ |  |  |
|  |  | eq. 3 | $\mathrm{P} / \mathrm{kPa}$ |  |  |
|  |  | A | 6.10462 |  |  |
|  |  | B | $1574.160$ |  |  |
|  |  | C | -67.079 |  |  |



FIGURE 4.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for indan.

### 4.1.1.2 Naphthalene



Common Name: Naphthalene
Synonym: naphthene, tar camphor, moth balls
Chemical Name: naphthalene
CAS Registry No: 91-20-3
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{8}$
Molecular Weight: 128.171
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
80.26 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
217.9 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.0253 (Weast 1983-84)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$125.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-from density)
133.2 (from density, Bohon \& Claussen 1951)
147.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Sublimation, $\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})$ :
73.93 (Colomina et al. 1982)
72.92 (Van Ekeren et al. 1983)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
19.29 (Parks \& Huffman 1931)
19.08 (Wauchope \& Getzen 1972; Podoll et al. 1989)
19.10 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
54.39 (Casellato et al. 1973)
54.81 (Ubbelohde 1978)
53.75, 44.4 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.287\left(\mathrm{mp}\right.$ at $80.26^{\circ} \mathrm{C}$ )
0.310 (calculated, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$, are compiled at the end of this section):
30.0* (shake flask-gravimetric, measured range $0-25^{\circ} \mathrm{C}$, Hilpert 1916)
31.5 (shake flask-UV, Andrews \& Keefer 1949)
12.5 (shake flask-UV, Klevens 1950)
34.4* (shake flask-UV, measured range $2-42^{\circ} \mathrm{C}$, Bohon \& Claussen 1951)
30.6 (Stephen \& Stephen 1963)
20.4 (shake flask, Sahyun 1966)
33.47 (shake flask-GC, Gordon \& Thorne 1967)
$38.4 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
31.2* (shake flask-UV, measured range $29-73.4^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-8690 /(\mathrm{T} / \mathrm{K})+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-13.4+0.0139 \cdot(\mathrm{~T} / \mathrm{K})$; temp range $29.2-73.4^{\circ} \mathrm{C}$ (shake
flask-UV, Wauchope \& Getzen 1972)
32.17 (shake flask-UV, Vesala 1974)
31.3 (shake flask-GC, Eganhouse \& Calder, 1976)
22.0 (fluorescence, Schwarz \& Wasik 1976)
31.7 (shake flask-fluorescence, Mackay \& Shiu, 1977)
30.0* $\quad\left(25^{\circ} \mathrm{C}\right.$, shake flask-fluorescence, measured range $8-31^{\circ} \mathrm{C}$, Schwarz \& Wasik 1977)
$30.25^{*} \quad\left(25^{\circ} \mathrm{C}\right.$, shake flask-fluorescence, measured range $8.4-31.8^{\circ} \mathrm{C}$, Schwarz 1977)
31.69 (generator column-HPLC/UV, measured temp range $5-30^{\circ} \mathrm{C}$, May et al. 1978)
$\mathrm{S} /(\mathrm{mg} / \mathrm{kg})=13.66+0.2499 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+0.0189 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}$; temp range $5-30^{\circ} \mathrm{C}$ (generator column-HPLC/UV, May et al. 1978)
30.64 (generator column-HPLC/UV, Wasik et al. 1983)
31.94* $\quad\left(25^{\circ} \mathrm{C}\right.$, generator column-HPLC/UV, measured range $8.2-27^{\circ} \mathrm{C}$, May et al. 1983)
$\mathrm{R} \cdot \ln x=-80.55 /(\theta / \mathrm{K})+28.7 /[1 /(\theta / \mathrm{K})-1 /(\mathrm{T} / \mathrm{K})]+0.31 \cdot\{(\theta / \mathrm{K}) /(\mathrm{T} / \mathrm{K})-1-\ln [(\theta / \mathrm{K}) /(\mathrm{T} / \mathrm{K})]\}, \theta=298.15 \mathrm{~K}$, temp range $8.2-27^{\circ} \mathrm{C}$ (generator column-HPLC/UV, May et al. 1983)
32.2 (average lit. value, Pearlman et al. 1984)
32.90 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
30.75* $\quad\left(25.2^{\circ} \mathrm{C}\right.$, shake flask-UV, Bennet \& Canady 1984)
$\ln x=-1767.4601 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})+(17.95209 / \mathrm{R}) \cdot \ln (\mathrm{T} / \mathrm{K})+1$; temp range $2-45^{\circ} \mathrm{C}$ (shake flask-UV, Bennet \& Canady 1984)
30.6 (shake flask-HPLC/UV, Fu \& Luthy 1985)
31.12 (vapor saturation-GC, Akiyoshi et al. 1987)
31.3, 31.9 (generator column-HPLC/UV, Billington et al. 1988)

31* (recommended, IUPAC Solubility Data Series, Shaw 1989)
33.71* (shake flask-UV, measured range $5-40^{\circ} \mathrm{C}$, Perez-Tejeda et al. 1990)
$\log \left[\mathrm{S} /\left(\mathrm{mol} / \mathrm{dm}^{3}\right)\right]=-31.24-143.5 /(\mathrm{T} / \mathrm{K})+4.772 \cdot \ln (\mathrm{~T} / \mathrm{K})$; temp range $5-40^{\circ} \mathrm{C}$ (shake flask-UV, Perez-Tejeda et al. 1990)
30.6 (generator column-HPLC, Vadas et al. 1991)
29.9 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
34.8 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=2.992-1001 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=-1.54117-3191.9 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$\log (\mathrm{P} / \mathrm{mmHg})=7.091-3465 /(\mathrm{T} / \mathrm{K})$; temp range $87-224$ (static isoteniscope method, Mortimer \& Murphy 1923) 8.64* $\quad\left(20^{\circ} \mathrm{C}\right.$, effusion, measured range $10-30^{\circ} \mathrm{C}$ Swan \& Mack 1925)
$\log (\mathrm{P} / \mathrm{mmHg})=29.820 /(\mathrm{T} / \mathrm{K})-200.682 \cdot \log (\mathrm{~T} / \mathrm{K})+595.642$; measured temp range $10-30^{\circ} \mathrm{C}$ (effusion, Swan \& Mack 1925)
$\log (\mathrm{P} / \mathrm{mmHg})=10.40-3429 /(\mathrm{T} / \mathrm{K})$; temp range $15-33^{\circ} \mathrm{C}$ (effusion, Zil'berman-Granovskaya 1940)
$133.3^{*} \quad\left(52.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $52.6-217.9^{\circ} \mathrm{C}$, Stull 1947)
14.26* (manometry-Rodebush gauge, Sears \& Hopke 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=-\left[108.30 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+27\right)\right]+1.115$; temp range $19-35^{\circ} \mathrm{C}$ (manometry-Rodebuch gauge, Sears \& Hopke 1949)
10.8* (effusion method, measured range $6.7-20.7^{\circ} \mathrm{C}$, Bradley \& Cleasby 1953)
$\log (\mathrm{P} / \mathrm{cmHg})=10.597-3783 /(\mathrm{T} / \mathrm{K})$; temp range $6.7-20.7^{\circ} \mathrm{C}$, (Antoine eq., effusion, Bradley \& Cleasby 1953)
$6815^{*} \quad\left(126.325^{\circ} \mathrm{C}\right.$, manometry, measured range $126.325-218.638^{\circ} \mathrm{C}$, Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.84577-1606.529 /\left(187.227+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $126.3-218.6^{\circ} \mathrm{C}$ (Antoine eq. Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=10.75-3616 /(\mathrm{T} / \mathrm{K})$; temp range -20 to $10^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958)
0.1188* $\quad\left(-13^{\circ} \mathrm{C}\right.$, Knudsen effusion, measured range -43 to $-13^{\circ} \mathrm{C}$, Miller 1963)
46.66* $\quad\left(40.33^{\circ} \mathrm{C}, \mathrm{Hg}\right.$ manometer, measured range $40.33-80.34^{\circ} \mathrm{C}$, Fowler et al. 1968)
10.98, 32.95 (manometry, extrapolated solid, supercooled liquid $P_{L}$, Fowler et al. 1968)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=9.58102-2692.92 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+220.651\right)$; temp range $40-80^{\circ} \mathrm{C}$ (Antoine eq., mercury manometer,
Fowler et al. 1968)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=7.03382-1756.91 /\left(\mathrm{t} /{ }^{\circ} \mathrm{C}+204.931\right)$; temp range $81-180^{\circ} \mathrm{C}$ (Antoine eq., mercury manometer,
Fowler et al. 1968)
30.66* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.01065-1733.71 /\left(201.859+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $86.581-250.27^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
11.60 (interpolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 17065.2 /(\mathrm{T} / \mathrm{K})]+11.450$; temp range $0-80.0^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 12311.6 /(\mathrm{T} / \mathrm{K})]+8.413089$; temp range $52.6-217.9^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
12.26* (Knudsen effusion method, extrapolated from measured data, Radchenko \& Kitiagorodskii 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=11.7041-3796.574 /(\mathrm{T} / \mathrm{K})$; temp range $9.0-23.91^{\circ} \mathrm{C}$ (Antoine eq., Knudsen effusion, Radchenko \& Kitiagorodskii 1974)
10.93* (gas saturation, Sinke 1974)
11.21* (Baratron model diaphragm pressure gauge, Ambrose et al. 1975)
$\mathrm{T} \cdot \log (\mathrm{P} / \mathrm{Pa})=1 / 2 \cdot a_{\mathrm{o}}+\sum a_{i} E_{i}(x) ; a_{\mathrm{o}}=310.6247, a_{1}=791.4937, a_{2}=-82536, a_{3}=0.4043$; temp range: 230-344 K, (Chebyshev polynomial, diaphragm pressure gauge, Ambrose et al. 1975)
$\log (\mathrm{P} / \mathrm{Pa}) 13.70-3773 /(\mathrm{T} / \mathrm{K})$ (Antoine eq. derived from exptl data of Ambrose et al. 1975, Wania et al. 1994) 13.5 (effusion method-pressure gauge, DePablo 1976)
10.64* (gas saturation, interpolated-Clapeyron eq., Macknick \& Prausnitz 1979)
$\log (\mathrm{P} / \mathrm{mmHg})=26.250-8575 /(\mathrm{T} / \mathrm{K})$; temp range $7.15-31.85^{\circ} \mathrm{C}$ (Clapeyron eq., gas saturation, Macknick \& Prausnitz 1979)
11.30* (effusion method, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=14.187-3907 /(\mathrm{T} / \mathrm{K})$; temp range $253-273 \mathrm{~K}$ (torsion effusion, regression, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=14.053-3860 /(\mathrm{T} / \mathrm{K})$; temp range $253-273 \mathrm{~K}$ (weighing effusion, regression, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=14.107-3886 /(\mathrm{T} / \mathrm{K})$; temp range $253-273 \mathrm{~K}$ (effusion, mean regression, de Kruif 1980)
10.42* (effusion method, de Kruif et al. 1981)
11.41* (Knudsen effusion, extrapolated-Antoine eq. from exptl data, Colomina et al. 1982)
$\log (\mathrm{P} / \mathrm{Pa})=14.01-3861.8 /(\mathrm{T} / \mathrm{K})$; temp range $271.46-284.63 \mathrm{~K}$ (Antoine eq., Knudsen effusion, Colomina et al. 1982) 11.33* (gas saturation-GC, Grayson \& Fosbraey 1982)
$\ln (\mathrm{P} / \mathrm{Pa})=31.8-8753 /(\mathrm{T} / \mathrm{K})$; temp range $302-352 \mathrm{~K}$, (Antoine eq., gas saturation, Grayson \& Fosbraey 1982) $\log (\mathrm{P} / \mathrm{atm})=[1-490.988 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.832267-4.41855 \times 10^{-4} .(\mathrm{T} / \mathrm{K})+2.89627 \times 10^{-7} .(\mathrm{T} / \mathrm{K})^{2}\right\} ;($ Cox eq., temp range $340.15-751.65 \mathrm{~K}$, Chao et al. 1983)
$6.53 \quad\left(20^{\circ} \mathrm{C}\right.$, Mackay et al. 1983)
10.4* (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=14.299-3960.03 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., gas saturation, Sonnefeld et al. 1983)
$1.63^{*} \quad\left(244.19^{\circ} \mathrm{C}\right.$, spinning-rotor gauge, measured range 244.19-255.86 K, Van Ekeren et al. 1983)
10.4 (generator column-HPLC, Wasik et al. 1983)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.93404-1579.278 /\left(184.062+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) ;$ temp range $126.3-218.6^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.1638-1760.018 /\left(215.204+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range $80.3-179.5^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
22.64, $28.24 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with BP-1 column, Apolane-87 column, Bidleman 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=7.01065-1733.71 /\left(201.86+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $86-250^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=6.8181-1585.86 /\left(184.82+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $125-218^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$10.7^{*} \quad\left(25.35^{\circ} \mathrm{C}\right.$, gas saturation, temp range $24.85-57.75^{\circ} \mathrm{C}$, Sato et al. 1986)
$\ln \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=22.8929-4025.35 /(\mathrm{T} / \mathrm{K}-102.243)$; temp range $298.5-330.9 \mathrm{~K}$ (Antoine eq., gas saturation, Sato et al. 1986)
11.27 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{S} / \mathrm{kPa}\right)=8.70592-2619.91 /(-52.499+\mathrm{T} / \mathrm{K})$; temp range $310-353 \mathrm{~K}$ (Antoine eq-I., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=9.45562-3069.145 /(-29.892+\mathrm{T} / \mathrm{K})$; temp range $263-353 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.9681-4577.47 /(30.394+\mathrm{T} / \mathrm{K})$; temp range not specified (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.19487-1782.509 /(-65.637+\mathrm{T} / \mathrm{K})$; temp range $352-500 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.14835-1751.644 /(-68.319+\mathrm{T} / \mathrm{K})$; temp range $491-565 \mathrm{~K}$ (Antoine eq.-V, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.53231-2162.182 /(-12.108+\mathrm{T} / \mathrm{K})$; temp range $563-665 \mathrm{~K}$ (Antoine eq.-VI, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.74783-4042.567 /(227.985+\mathrm{T} / \mathrm{K})$; temp range $661-750 \mathrm{~K}$ (Antoine eq.-VII, Stephenson \& Malanowski 1987)
11.37* (pressure gauge, interpolated-Antoine eq., measured range -12.15 to $70.16^{\circ} \mathrm{C}$, Sasse et al. 1988) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=10.05263-2907.918 /\left(236.459+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -12.15 to $70.16^{\circ} \mathrm{C}$ (Antoine eq., pressure gauge, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=2.25180-76.496 /\left(-25.09+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $80.16-90.15^{\circ} \mathrm{C}$ (Antoine eq., pressure gauge, Sasse et al. 1988)
22.65 (PGC, GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
41.88, 38.02 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ values converted from literature $\mathrm{P}_{\mathrm{S}}$ with different $\Delta \mathrm{S}_{\text {fus }}$ values, Hinckley et al. 1990)
$0.7634^{*} \quad\left(0^{\circ} \mathrm{C}\right.$, gas saturation-GC, measured range -30.6 to $0^{\circ} \mathrm{C}$, Wania et al. 1994)
$\log (\mathrm{P} / \mathrm{Pa})=13.93-3851 /(\mathrm{T} / \mathrm{K})$; temp range -30 to $0^{\circ} \mathrm{C}$, (Antoine eq., gas saturation, Wania et al. 1994)
24.0 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation, Donovan 1996)
5.58-12.30; 10.4-14.0; 11.2-14.4; 7.71-17.2; 6.45-8.40 (quoted lit. ranges: effusion method; gas saturation; manometry; calculated; from GC-RT correlation, Delle Site 1997)
11.16 (solid $\mathrm{P}_{\mathrm{S}}$, van der Linde et al. 1998)
40.0; 12.4 (quoted $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F , Passivirta et al. 1999) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=10.90-2927 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=8.06-1923 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{Pa})=13.59-3742 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
37.0 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-2930 /(\mathrm{T} / \mathrm{K})+11.39 ; \Delta \mathrm{H}_{\text {vap }} .=-56.1 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
56.0 (gas stripping, Southworth, 1979)
48.9 (gas stripping, Mackay et al. 1979; Mackay \& Shiu 1981)
44.6 (gas stripping, Mackay et al. 1982)
$36.5 \quad\left(20^{\circ} \mathrm{C}\right.$, EPICS method, Yurteri et al. 1987)
74.3 (wetted-wall column-GC, Fendinger \& Glotfelty 1990)

124 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
47.1 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
42.6* (gas stripping-GC, measured range $3.7-35.5^{\circ} \mathrm{C}$, Alaee et al. 1996)
$\ln \mathrm{K}_{\mathrm{AW}}=13.95-5364.45 /(\mathrm{T} / \mathrm{K})$, temp range: $3.7-35.5^{\circ} \mathrm{C}$ (gas stripping-GC, Alaee et al. 1996)
$26.2,35.5,48.1,62.5,77.7,108.1\left(9.2,14.5,20.1,24.6,30.5,34.8^{\circ} \mathrm{C}\right.$, seawater with salinity of $351 \%(0.660 \mathrm{M}$ NaCl ), gas stripping-GC, Alaee et al. 1996)
44.6 (gas stripping-GC; calculated-P/C, Shiu \& Mackay 1997)
45.0 (gas stripping-HPLC/fluo., De Maagd et al. 1998)
57.0 (gas stripping-GC, Altschuh et al. 1999)
$\log \mathrm{K}_{\mathrm{AW}}=6.058-2332 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
3.37
3.37, 3.01, 3.45
3.37
3.395
3.36
3.35; 3.42
3.57
3.38
3.43
3.30, 3.01, 3.37, 3.45, $3.59 \quad$ (quoted, Hansch \& Leo 1979)
3.17 (HPLC-RT correlation, Veith et al. 1979a,b)
3.36 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
3.21 (HPLC-k' correlation, Hanai et al. 1981)
3.18 (HPLC-k' correlation, D'Amboise \& Hanai 1981)
3.35 (generator column-HPLC/UV, Wasik et al. 1981 1983)
3.35 (RP-TLC-k' correlation, Bruggeman et al. 1982)
3.45 (HPLC-RT correlation, Hammers et al. 1982)
3.31; 3.35 (shake flask; HPLC correlation, Eadsforth \& Moser 1983)
(shake flask, Fujita et al. 1964; Hansch et al. 1973)
(Leo et al. 1971)
(calculated-fragment const., Rekker 1977)
(shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
(generator column-HPLC/UV, Wasik et al. 1981 1983)
(HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
(shake flask; ALPM, Garst \& Wilson 1984)
(HPLC-RV correlation, Garst \& Wilson 1984)
(RP-HPLC correlation, Chin et al. 1986)
(HPLC-RT correlation, Edsforth 1986)
3.29
(HPLC-RT correlation, Wang et al. 1986)
(HPLC-RT correlation, de Kock \& Lord 1987)
(average, HPLC-RT correlation, Ge et al. 1987)
(shake flask-GC, Opperhuizen et al. 1987)
(HPLC-RT correlation, Minick et al. 1988)
(RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
(recommended, Sangster 1989, 1993)
(centrifugal partition chromatography, Menges et al. 1990)
(shake flask-HPLC/UV, Menges \& Armstrong 1991)
(TLC-RT correlation, De Voogt et al. 1990)
(centrifugal partition chromatography, Berthod et al. 1992)
(shake flask-UV, pH 7.4, Alcorn et al. 1993)
(recommended, Hansch et al. 1995)
$\left(26^{\circ} \mathrm{C} ; 4^{\circ} \mathrm{C}\right.$, quoted, Piatt et al. 1996)
(HPLC-k' correlation: ODS column; Diol column; quoted lit. average, Helweg et al. 1997) (range 3.24-3.40) (slow stirring method-HPLC/fluo., De Maagd et al. 1998)
(shake flask-dialysis tubing-HPLC/UV, both phases, Andersson \& Schrăder 1999)
(RP-HPLC-RT correlation, short ODP column, Donovan \& Pescatore 2002)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ :
5.10 (calculated- $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, Wania \& Mackay 1996)
5.19 (calculated- $\mathrm{S}_{\text {oct }}$ and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ at $25^{\circ} \mathrm{C}$ :

| 1.64 | (mussel Mytilus edulis, Lee et al. 1972) |
| :--- | :--- |
| 4.11 | (bile of rainbow trout, Melancon \& Lech 1978) |
| 2.12 | (Daphnia pulex, Southworth et al. 1978) |
| 2.07 | (Daphnia pulex, by kinetic estimation, Southworth et al. 1978) |
| 2.63 | (fathead minnow, Veith et al. 1979b, 1980) |
| 2.62 | (microorganisms-water, calculated from K K |
| $4.10,3.84,4.25$ | (average, Selenastrum capricornutum-dosed singly, dosed simultaneously, Casserly et al. |
|  | 1983) |
| $2.11 ; 2.43$ | (Chlorella fusca; calculated-K |
| $1.48,2.10,3.0$ | (fish, algae, activated sludge, Freitag et al. 1985) |
| 2.50 | (bluegill sunfish, McCarthy \& Jimenez 1985) |
| 2.48 | (bluegill sunfish with dissolved humic material, McCarthy \& Jimenez 1985) |

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
3.11 (natural sediment, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
$2.38 \quad\left(22^{\circ} \mathrm{C}\right.$, suspended particulates, Herbes et al. 1980)
2.94 (sediment/soil, sorption isotherm by batch equilibrium, Karickhoff 1981)
3.62, $3.87,4.23$ (soil I-very strongly acid sandy soil pH 4.5-5.5, soil II-moderately or slightly acid loamy
soil $\mathrm{pH} 5.6-6.5$, soil III-slightly alkaline loamy soil pH 7.1-8.0, OECD 1981)
3.50; 4.43; 3.21 (Speyer soils: $\mathrm{pH} 7.0,0.69 \%$ OC; pH 5.8, $2.24 \%$ OC; pH $7.1,1.12 \%$ OC at $0.15-0.5 \mathrm{~mm}$, batch equilibrium-sorption isotherm, Rippen et al. 1982)
$3.11 ; 3.16$ (soils: Alfisol $0.76 \% \mathrm{OC}$ at pH 7.5 , Entisol $1.11 \% \mathrm{OC}$ at pH 7.9 , batch equilibrium-sorption isotherm, Rippen et al. 1982)
3.30 (Offshore Grand Haven sediment, batch equilibrium-sorption isotherm, Voice \& Weber 1985)
2.67, 2.77 (Lula aquifer 0.032\% OC, Apalachee soil $1.4 \%$ OC, batch equilibrium-sorption isotherm, Stauffer \& MacIntyre 1986)
2.95 (sediment, calculated, Pavlou 1987)
2.93 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
3.27 (calculated-MCI $\chi$, Bahnick \& Doucette 1988)
3.02; 2.89 (Aldrich and Fluka humic acid, observed; predicted, Chin et al. 1989)
2.73-3.91 (aquifer materials, Stauffer et al. 1989)
5.00 (sediments average, Kayal \& Connell 1990)
3.15, 2.76 (Menlo Park soil, Eustis sand, batch equilibrium-sorption isotherm, Podoll et al. 1989)
$3.21,3.16,3.10,3.00\left(15,25,35,50^{\circ} \mathrm{C}\right.$, Menlo Park soil $1.6 \%$ OC, flow sorption equilibrium, Podoll et al. 1989)
2.97, 2.67 (modified, unmodified EPA-6 sediments, batch equilibrium-sorption isotherm, Podoll et al. 1989)
3.11 (soil, RP-HPLC-k' correlation, Szabo et al. 1990a)
3.29 (sandy surface soil, Wood et al. 1990)
2.97 (dissolved organic matter, Kan \& Tomson 1990)
2.98; 2.965, 2.98 (sediment: conen ratio $\mathrm{C}_{\text {sed }} / \mathrm{C}_{\mathrm{w}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter \& Alden 1994)
3.11 (calculated-MCI ${ }^{1} \chi$, Sabljic et al. 1995)
3.16, 3.05, 3.06 (RP-HPLC-k' correlation on different stationary phases, Szabo et al. 1995)
2.75 (HPLC-screening method; Müller \& Kördel 1996)
4.06 (range 3.95-4.15); 2.08 (range $2.08-2.11)\left(4^{\circ} \mathrm{C}\right.$, low organic carbon sediment $\mathrm{f}_{\text {OC }}=0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
3.90 (range 3.81-4.00); 2.11 (range 2.11-2.13) $\left(26^{\circ} \mathrm{C}\right.$, low organic carbon sediment $\mathrm{f}_{\mathrm{OC}}=0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
3.74 (humic acid, HPLC-k' correlation; Nielsen et al. 1997)
2.42-2.56 (5 soils, $20^{\circ} \mathrm{C}$, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
$2.61,2.63,2.68,2.77,2.76$, mean $2.69 \pm 0.073$ (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choiu et al. 1998)
2.91, 2.86, 2.88, 2.87, 2.89, 2.95, 3.07; mean $2.88 \pm 0.22$ (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choiu et al. 1998)
3.11 (3.00-3.19), 2.80 (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
3.60; 3.10 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
3.09-5.51; 2.60-5.0 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$3.91 ; 4.12,4.06,4.94\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)
2.91, 3.02, 2.71 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%, \mathrm{OC} \geq 0.5 \%, 0.1 \leq \mathrm{OC}<0.5 \%$, average, Delle Site 2001)
3.06 (average values for sediments OC $\geq 0.5 \%$, Delle Site 2001)
4.43 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Environmental Fate Rate Constants, $k$, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization/Evaporation: rate of evaporation estimated to be $1.675 \times 10^{-9} \mathrm{~mol} \mathrm{~cm}^{-2} \mathrm{~h}^{-1}$ at $20^{\circ} \mathrm{C}$ and air flow rate of $50 \mathrm{~L} \mathrm{~h}^{-1}$ (Gückel et al. 1973);
calculated $t_{1 / 2}=7.15 \mathrm{~h}$ from 1 m depth of water (Mackay \& Leinonen 1975; quoted, Haque et al. 1980);
$t_{1 / 2}=16 \mathrm{~h}$ for surface waters for a river 1-m deep, water velocity $0.5 \mathrm{~m} / \mathrm{s}$, wind velocity $1 \mathrm{~m} / \mathrm{s}$ (Southworth
1979; Herbes et al. 1980);
evaporation $t_{1 / 2}=50 \mathrm{~h}$ in a river and $t_{1 / 2}=200 \mathrm{~h}$ in a lake when considering current velocity and wind speed in combined with typical reaeration rates for natural bodies of water (Howard 1989);
$\mathrm{t}_{1 / 2}($ exptl $)=28 \mathrm{~min}$ and $\mathrm{t}_{1 / 2}($ calc $)=32 \mathrm{~min}$ from solution (Mackay et al. 1983).
Photolysis:
$t_{1 / 2}=71 \mathrm{~h}$ calculated for direct photochemical transformation near-surface water and $\mathrm{t}_{1 / 2}=550 \mathrm{~d}$ in $5-\mathrm{m}$ deep inland water body at $40^{\circ} \mathrm{N}$ at midday of midsummer (Zepp \& Schlotzhauer 1979)
$\mathrm{k}=0.0392 \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with HO - in the gas (Dilling et al. 1988)
$\mathrm{k}=0.028 \mathrm{~h}^{-1}$ in distilled water with $\mathrm{t}_{1 / 2}=25 \mathrm{~h}$ (Fukuda et al. 1988)
$\mathrm{k}=6.0 \times 10^{-4} \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=19.18 \mathrm{~h}$, photodegradation in methanol-water ( $3: 7, \mathrm{v} / \mathrm{v}$ ) solution with initial concentration of 50.0 ppm by high-pressure mercury lamp or sunlight (Wang et al. 1991);
$\mathrm{k}($ exptl $)=0.000511 \mathrm{~min}^{-1}$ with $\mathrm{t}_{1 / 2}($ calc $)=22.61 \mathrm{~h}$ and the predicted $\mathrm{k}=0.000303 \mathrm{~min}^{-1}$ by QSPR, the pseudo-first-order direct photolysis rate constant of in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
$\mathrm{t}_{1 / 2}($ calc $)=15.42 \mathrm{~h}$ direct photolysis half-life in atmospheric aerosol (QSPR, Chen et al. 2001).
Oxidation: rate constant k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated; *data at other temperatures and/or Arrhenius equation see reference:
k (calc) $<360 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen, $\mathrm{k}\left(\right.$ calc) $<1 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=(2.42 \pm 0.19) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with an estimated atmospheric lifetime $\tau \sim 1 \mathrm{~d}$, and $\mathrm{k}_{\mathrm{O}_{3}}<$ $2 \times 10^{-9} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} 294 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al 1984)
$\mathrm{k}_{\mathrm{OH}}=(2.35 \pm 0.06) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 1 \mathrm{~K}$ (relative rate method, Biermann et al. 1985)
$\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}} \sim(2-3) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ at 298 K , the calculated lifetime $\tau-10 \mathrm{~d}$ due to night-time reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ in atmosphere (relative rate method, Pitts et al. 1985)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=2.17 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}=(2.59 \pm 0.24) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a lifetime of $\sim 11 \mathrm{~h}, \mathrm{k}_{\mathrm{O}_{3}}<3 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson \& Aschmann 1986)
$\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=(1.4 \pm 0.2) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{N}_{2} \mathrm{O}_{5}$ at 298 K (relative rate method, Atkinson et al. 1987)
$\mathrm{k}_{\mathrm{OH}}=2.17 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O}_{3}}<2 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, and $\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=1.4 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{N}_{2} \mathrm{O}_{5}$ at room temp. (Atkinson \& Aschmann 1987, 1988)
$\mathrm{k}_{\mathrm{OH}}=(22.8-25.9) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 294-298 K (review, Atkinson 1989)
$\mathrm{k}_{\mathrm{oH}}{ }^{*}=2.16 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=26.58 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=23 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $306-366 \mathrm{~K}$ with a calculated atmospheric lifetime of 12 h based on gas-phase OH reaction (Brubaker \& Hites 1998)
$\mathrm{k}_{\mathrm{OH}}=(2.39 \pm 0.09) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$, with a calculated tropospheric lifetime of 5.8 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Hydrolysis: not hydrolyzable (Mabey et al. 1982).
Biodegradation:
$\mathrm{k}=4 \times 10^{-6} \mathrm{~g} \mathrm{~L}^{-1} \mathrm{~d}^{-1}$ ultimate loss process (Lee \& Ryan, 1976)
$\mathrm{k}=(0.04-3.3) \times 10^{-6} \mathrm{~g} \mathrm{~L}^{-1} \mathrm{~d}^{-1}$ (Lee \& Anderson 1977)
complete degradation in 8 d in gas-oil contaminated groundwater which was circulated through sand that had been inoculated with groundwater under aerobic conditions (Kappeler \& Wuhrmann 1978; quoted, Howard 1989)
$\mathrm{k}=0.04-3 \mu \mathrm{~g} / \mathrm{L} \mathrm{d}$ for microorganisms (Callahan et al. 1979)
$t_{1 / 2}=1.9 \mathrm{~d}$, in deeper and slowly moving contaminated water (Herbes 1981; Wakeham et al. 1983; quoted, Howard 1989);
half-lives: of $7,24,63$ and 1700 d in an oil polluted estuarine stream, clean estuarine stream, coastal waters, and in the Gulf stream, respectively (Lee 1977; quoted, Howard 1989)
$\mathrm{t}_{1 / 2}($ aerobic $)=12 \mathrm{~h}$, based on die-away test data for an oil polluted creek (Walker \& Colwell 1976)
$\mathrm{t}_{1 / 2}=480 \mathrm{~h}$, for an estuarine river (Lee \& Ryan 1976).
$\mathrm{t}_{1 / 2}($ anaerobic $)=25 \mathrm{~d}$ at pH 8 and $\mathrm{t}_{1 / 2}=258 \mathrm{~d}$ at pH 5 (Hambrick et al. 1980);
$\mathrm{t}_{1 / 2}=1.9 \mathrm{~d}$, in deeper and slower moving contaminated water (Herbes 1981; Wakeham et al. 1983)
$\mathrm{k}=0.23 \mathrm{~h}^{-1}$ (microbial degradation rate constant, Herbes et al. 1980, Hallett \& Brecher 1984)
$100 \%$ degradation within 7 d for an average of three static-flask screening test (Tabak et al. 1981)
$\mathrm{k}=3.2 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=9 \mathrm{~h} ; \mathrm{k}=7.6 \times 10^{-2} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=9 \mathrm{~h}$ for mixed bacterial populations in water and sediment from the same stream (NRCC 1983)
$\mathrm{k}=0.14 \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=5 \mathrm{~h} ; \mathrm{k}<4 \times 10^{-4} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}>72 \mathrm{~d}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)
degraded completely within 1 wk by microbes in non-autoclaved samples of $0.04 \mathrm{mg} / \mathrm{L}$ in groundwater from hazardous waste site (Lee et al. 1984)
$\mathrm{k}=0.024 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=28 \mathrm{~d}$ in groundwater with nutrients and acclimated microbes, $\mathrm{k}=0.013 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}$ $=53 \mathrm{~d}$ in river water with acclimated microbes, and $\mathrm{k}=0.018 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=39 \mathrm{~d}$ in river water with nutrients and acclimated microbes (Vaishnav \& Babeu 1987)
$\mathrm{k}=0.337 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.1 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.308 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.2 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
$\mathrm{t}_{1 / 2}($ aerobic $)=12-480 \mathrm{~h}$, based on die-away test data and for estuarine river (Howard et al. 1991)
$t_{1 / 2}($ anaerobic $)=500-6192 \mathrm{~h}$, based on anaerobic estuarine sediment die-away test data (Howard et al. 1991) removal rate of 2.4 and 0.43 mg ( g of volatile suspended solid d$)^{-1}$, degradation by bacteria from creosotecontaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne \& Strand 1998)
Biotransformation: estimated rate constant for bacteria, $1 \times 10^{-7} \mathrm{ml} \mathrm{cell}^{-1} \mathrm{~h}^{-1}$ (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) or Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=197 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=1.667 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978; quoted, Hawker \& Connell 1986)
$\log \mathrm{k}_{2}=-0.70,-1.70 \mathrm{~d}^{-1}$ (fish, calculated- $\mathrm{K}_{\mathrm{OW}}$, Thomann 1989)
Half-Lives in the Environment:
Air: volatility of $2.28 \times 10^{4} \mathrm{~s}$ (experimental), $7.7 \times 10^{3} \mathrm{~s}$ (calculated) for depth of water body of $22.5 \mathrm{~m}\left(23^{\circ} \mathrm{C}\right.$,
Klöpffer et al. 1982);
estimated lifetime of $\sim 1 d$ due to reaction with photochemically produced hydroxyl radical, assuming an average daytime atmospheric OH radical concn of $\sim 1 \times 10^{6}$ molecule/cm ${ }^{3}$ (Atkinson et al. 1984, 1987; quoted, Howard 1989);
calculated lifetime of $\sim 11 \mathrm{~h}$ due to reaction with OH radical (Atkinson \& Aschmann 1986);
the atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radical and with $\mathrm{N}_{2} \mathrm{O}_{5}$ can be calculated to range from $\sim 4$ to 13 h and $20-80 \mathrm{~d}$, respectively (Atkinson \& Aschmann 1987);
$t_{1 / 2}=2.96-29.6 \mathrm{~h}$ based on photooxidation half-life in air (Howard et al. 1991);
calculated atmospheric lifetime of 12 h based on gas-phase OH reactions (Brubaker \& Hites 1998).
Surface Water: $t_{1 / 2}=16 \mathrm{~h}$ (calculated for river water 1 m deep, water velocity $0.5 \mathrm{~m} / \mathrm{s}$, wind velocity $1 \mathrm{~m} / \mathrm{s}$ from air-water partition coefficients (Southworth 1979; Hallett \& Brecher 1984)
$t_{1 / 2}=71 \mathrm{~h}$ of photolysis in near surface water, but $t_{1 / 2}=550 \mathrm{~d}$ for a depth of 5 m (calculated from surface water in midsummer at $40^{\circ} \mathrm{N}$ latitude, Zepp \& Schlotzhauer 1979);
calculated $t_{1 / 2}=7.15 \mathrm{~h}$, based on evaporative loss for a water depth of 1 m at $25^{\circ} \mathrm{C}$ (Mackay \& Leinonen 1975); an overall $\mathrm{t}_{1 / 2}=2.3 \mathrm{~d}$ in Rhine river based on monitoring data (Zoeteman et al. 1980)
in coastal seawater mesocosm experiments: $\mathrm{k}=0.058 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=12 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ during the periods when volatilization dominates, $\mathrm{k}=0.061 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=11.3 \mathrm{~h}$ with $\mathrm{HgCl}_{2}$ as poison and $\mathrm{k}=0.896$ $\mathrm{d}^{-1}$ corresponding to $\mathrm{t}_{1 / 2}=0.8 \mathrm{~h}$ without poison (Wakeham et al. 1983);
$\mathrm{t}_{1 / 2}=12-480 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); photolysis $t_{1 / 2}=22.81 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater: estimated $\mathrm{t}_{1 / 2}=0.6 \mathrm{yr}$ in the Netherlands (Zoeteman et al. 1981);
$t_{1 / 2}=24-6193 \mathrm{~h}$ based on estimated unacclimated aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).
Sediment: $t_{1 / 2}=4.9 \mathrm{~h}$ in oil contaminated sediment and $\mathrm{t}_{1 / 2}>88 \mathrm{~d}$ in uncontaminated sediments (Herbes \& Schwall 1978; quoted, Howard 1989);
desorption $\mathrm{k}=0.031 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=21.3 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: an overall $t_{1 / 2}=3.6$ months in a solid waste site (Zoeteman et al. 1981);
$\mathrm{t}_{1 / 2}=0.12-125 \mathrm{~d}$ (Sims \& Overcash 1983);
$\mathrm{t}_{1 / 2}=12 \mathrm{~d}$ for both $5 \mathrm{mg} / \mathrm{kg}$ and $50 \mathrm{mg} / \mathrm{kg}$ added (Bulman et al. 1987);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
$\mathrm{t}_{1 / 2}>80 \mathrm{~d}$ (Howard 1989);
biodegradation $\mathrm{k}=0.337 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.1 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{k}=0.308 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.2 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$t_{1 / 2}=398-1152 \mathrm{~h}$, based on soil-die-away test data (Howard et al. 1991); $\mathrm{t}_{1 / 2}=0.02-46 \mathrm{wk}, \mathrm{t}_{1 / 2}<2.1 \mathrm{yr}$ (quoted, Ludington soil, Wild et al. 1991).
Biota: elimination half-lives $\mathrm{t}_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes, $\mathrm{t}_{1 / 2}=2.0 \mathrm{~d}$ from clam Macoma balthica quoted, Meador et al. 1995).

TABLE 4.1.1.2.1
Reported aqueous solubilities of naphthalene at various temperatures and empirical temperature dependence equations

$$
\begin{align*}
& \mathrm{R} \cdot \ln x=-\Delta \mathrm{H}_{\mathrm{fus}} /(\mathrm{T} / \mathrm{K})+(0.000408) \cdot[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{~T} / \mathrm{K})  \tag{1}\\
& \mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}_{1 / 2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}  \tag{2}\\
& \mathrm{R} \cdot \ln x=-30.55 / \theta+28.7 /(1 / \theta-1 / \mathrm{T})+0.31[\theta / \mathrm{T}-1-\ln (\theta / \mathrm{T})]  \tag{3}\\
& \ln x=1767.460 /[\mathrm{R} \cdot(\mathrm{~T} / \mathrm{K})]+(17.95209 / \mathrm{R}) \cdot \ln (\mathrm{T} / \mathrm{K})+1  \tag{4}\\
& \log \left(\mathrm{~S} / \mathrm{mol} \cdot \mathrm{dm}^{-3}\right)=-31.24-143.5 /(\mathrm{T} / \mathrm{K})+4.772 \cdot \ln (\mathrm{~T} / \mathrm{K}) \tag{5}
\end{align*}
$$

1. 

| Hilpert 1916 |  | Bohon \& Claussen 1951 |  | Wauchope \& Getzen 1972 |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-gravimetry |  | shake flask-UV |  | shake flask-UV |  |  |  |
| $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ}{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  |  |  |  |  | exptl. |  | smoothed |
| 0 | 19 | 25 | 34.4 | 22.2 | 28.8 | 0 | 13.7 |
| 25 | 30 | 0 | 13.74 | 22.2 | 29.1 | 22.2 | 28.3 |
|  |  | 0.4 | 13.74 | 24.5 | 30.8 | 24.5 | 30.7 |
|  |  | 0.5 | 13.85 | 24.5 | 30.1 | 25.0 | 31.2 |
|  |  | 0.9 | 14.59 | 24.5 | 30.7 | 29.9 | 37.3 |
|  |  | 9.4 | 19.62 | 29.9 | 38.1 | 30.3 | 37.8 |
|  |  | 10 | 19.42 | 29.9 | 38.2 | 34.5 | 44.3 |
|  |  | 14.9 | 23.43 | 29.9 | 38.3 | 39.3 | 53.3 |
|  |  | 15.9 | 24.56 | 30.3 | 38.1,37.6 | 40.1 | 55.0 |
|  |  | 19.3 | 28.05 | 34.5 | 44.6,43.8 | 44.7 | 66.2 |
|  |  | 25.6 | 36.6 | 39.3 | 52.6, 52.8 | 50.0 | 82.4 |
|  |  | 30.1 | 42.97 | 40.1 | 54.8 | 50.2 | 83.1 |
|  |  | 30.2 | 43.87 | 44.7 | 66.0 | 55.6 | 105 |
|  |  | 35.2 | 54.45 | 44.7 | 65.5 | 64.5 | 156 |
|  |  | 36.0 | 54.81 | 44.7 | 65.3 | 73.4 | 239 |
|  |  | 42.8 | 73.49 | 50.2 | 78.6 | 75 | 258 |
|  |  |  |  | 55.6 | 106 |  |  |
|  |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |  | 64.5 | 166 | temp de | dence eq. 1 |
|  |  | $2^{\circ} \mathrm{C}$ | 4.14 | 64.5 | 151 | $\ln \mathrm{X}$ | mole fraction |
|  |  | $7^{\circ} \mathrm{C}$ | 5.77 | 64.5 | 157 | $\Delta \mathrm{H}_{\text {fus }}=$ | $36.36 \pm 0.17$ |
|  |  | $12^{\circ} \mathrm{C}$ | 7.24 | 73.4 | 240 | $10^{2} \cdot \mathrm{~b}$ | $1.39 \pm 0.05$ |
|  |  | $17^{\circ} \mathrm{C}$ | 8.49 | 73.4 | 247 | c | $13.4 \pm 0.2$ |
|  |  | $22^{\circ} \mathrm{C}$ | 10.17 | 73.4 | 244 |  |  |
|  |  | $27^{\circ} \mathrm{C}$ | 12.80 |  |  |  |  |
|  |  | $32^{\circ} \mathrm{C}$ | 14.23 | $\Delta \mathrm{H}_{\text {fus }} /$ | $=36.36$ |  |  |
|  |  | $37^{\circ} \mathrm{C}$ | 15.69 |  |  |  |  |

TABLE 4.1.1.2.1 (Continued)
2.

3.



FIGURE 4.1.1.2.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for naphthalene.

## TABLE 4.1.1.2.2

Reported vapor pressures of naphthalene at various temperatures and coefficients for vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
(3)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
1.

| Swan \& Mack 1925 |  | Stull 1947 |  | Sears \& Hopke 1949 |  | Bradley \& Cleasby 1953 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| effusion |  | summary of literature data |  | manometry |  | effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 10 | 2.32 | 52.6 | 133.3 | 10 | 2.053 | 6.7 | 1.627 |
| 20 | 8.64 | 74.2 | 666.6 | 20 | 8.533 | 8.1 | 1.88 |
| 30 | 23.60 | 85.8 | 1333 | 30 | 21.87 | 12.3 | 2.96 |
|  |  | 101.7 | 2666 |  |  | 12.7 | 3.13 |
| eq. 4 | $\mathrm{P} / \mathrm{mmHg}$ | 119.3 | 5333 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 13.85 | 3.506 |
| A | 595.642 | 130.2 | 7999 | A | 1.115 | 15.65 | 4.266 |
| B | 29.820 | 145.5 | 13332 | B | 108.3 | 16.85 | 4.67 |
| C | 200.682 | 167.7 | 26664 | C | 27 | 17.35 | 5.09 |
|  |  | 193.2 | 53329 |  |  | 18.7 | 5.106 |
|  |  | 217.9 | 101325 |  |  | 20.7 | 7.12 |
|  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 80.2 |  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 10.597 |
|  |  |  |  |  |  | B | 3783 |

(Continued)

TABLE 4.1.1.2.2 (Continued)
2.

3.

| Sinke 1974 |  | Radchenko \& K. 1974 |  | Ambrose 1975 |  | Macknick \& Prausnitz 1979 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation |  | effusion |  | diaphragm gauge |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| -53.15 | 0.00028 | 9.0 | 2.357 | 263.61 | 0.23 | 7.15 | 1.76 |
| -33.15 | 0.00837 | 10.7 | 3.113 | 267.98 | 0.40 | 12.8 | 3.133 |
| -13.15 | 0.144 | 12.5 | 5.637 | 273.16 | 0.74 | 18.4 | 5.586 |
| 6.85 | 1.631 | 14.4 | 7.546 | 278.22 | 1.38 | 18.85 | 5.933 |
| 25 | 10.93 | 16.3 | 19.59 | 283.14 | 2.41 | 26.4 | 12.58 |
| 26.85 | 13.092 | 18.2 | 31.09 | 288.01 | 4.13 | 31.85 | 20.53 |
| 46.85 | 79.73 | 20.0 | 48.37 | 288.01 | 4.17 | 25 | 10.64 |
| 66.85 | 386.5 | 21.95 | 74.19 | 293.24 | 6.93 |  |  |
| 80.28 | 999.8 | 23.91 | 112.6 | 293.25 | 6.95 | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | 25 | 12.26* | 298.26 | 11.35 | A | 26.25 |
| eq. 1 | $\mathrm{P} / \mathrm{Pa}$ |  |  | 303.29 | 18.45 | B | 8575 |
| A | 13.83 | $\Delta \mathrm{H}_{\text {subl }} / \mathrm{kJ} \mathrm{mol}^{-1}=72.72$ |  | 308.17 | 28.95 |  |  |
| B | 3817 |  | at $25^{\circ} \mathrm{C}$ | 313.24 | 44.73 |  |  |

TABLE 4.1.1.2.2 (Continued)

| Sinke 1974 |  | Radchenko \& K. 1974 |  | Ambrose 1975 |  | Macknick \& Prausnitz 1979 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation |  | effusion |  | diaphragm gauge |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  |  |  | 318.21 | 68.82 |  |  |
|  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | 323.14 | 104.14 |  |  |
|  |  | A | 11.7041 | 328.24 | 158.41 |  |  |
|  |  | B | 3798.574 | 333.39 | 237.54 |  |  |
|  |  | *calc | g eq. 1 | 333.34 | 238.73 |  |  |
|  |  |  |  | 333.34 | 238.47 |  |  |
|  |  |  |  | 338.10 | 340.58 |  |  |
|  |  |  |  | 343.06 | 488.58 |  |  |
|  |  |  |  | $\begin{aligned} & \Delta \mathrm{H}_{\text {sub }} / \mathrm{KJ} \mathrm{~mol}-1=72.5 \\ & \text { at } 25^{\circ} \mathrm{C} \end{aligned}$ |  |  |  |

4. 

| de Kru |  | de Kruif et al. 1981 |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| torsion-effusion |  | diaphragm gauge |  |  |  |  |  |
| T/K | P/Pa | T/K | P/Pa | T/K | $\mathrm{P} / \mathrm{Pa}$ | T/K | P/Pa |
|  |  | solid |  | cont'd |  |  |  |
| 257.21 | 0.1 | 274.44 | 0.87 | 340.92 | 421.8 | liquid |  |
| 262.44 | 0.2 | 276.40 | 1.10 | 348.82 | 717.5 | 355.23 | 1069 |
| 265.59 | 0.3 | 279.12 | 1.50 | 350.44 | 790.2 | 356.83 | 1155 |
| 267.88 | 0.4 | 280.62 | 1.78 | 352.44 | 914.5 | 359.78 | 1328 |
| 269.68 | 0.5 | 282.73 | 2.24 | 344.72 | 538.0 | 362.77 | 1526 |
| 271.17 | 0.6 | 285.37 | 3.07 | 345.76 | 586.6 | 355.38 | 1083 |
| 272.44 | 0.7 | 285.71 | 3.11 | 328.79 | 159.2 | 372.05 | 2305 |
| 273.56 | 0.8 | 287.98 | 3.98 | 324.57 | 118.5 | 377.33 | 2899 |
| 274.55 | 0.9 | 288.11 | 4.02 | 345.92 | 580.4 | 385.20 | 4006 |
| 275.44 | 1.0 | 290.46 | 5.16 | 324.87 | 121.9 | 381.92 | 3504 |
|  |  | 290.88 | 5.35 | 347.53 | 650.0 | 372.45 | 2351 |
| $\Delta \mathrm{H}_{\text {subl }} / \mathrm{kJ} \mathrm{mol}^{-1}=$ |  | 292.75 | 6.53 | 347.57 | 653.9 | 368.07 | 1929 |
| 298.15 K | 72.6 | 320.34 | 83.91 | 344.72 | 547.1 | 363.74 | 1591 |
| 253-273 K | 74.4 | 319.87 | 80.76 | 344.86 | 549.1 | 353.57 | 982 |
|  |  | 275.50 | 0.99 | 352.00 | 901.3 | 357.10 | 1176 |
|  |  | 282.12 | 2.10 | 319.58 | 78.38 | 361.10 | 1423 |
|  |  | 277.86 | 1.30 | 319.59 | 77.9 | 367.72 | 1926 |
|  |  | 325.41 | 126.7 | 325.96 | 132.1 | 380.51 | 3355 |
|  |  | 288.51 | 4.22 | 341.26 | 419.9 | 388.20 | 4545 |
|  |  | 293.83 | 7.29 | 349.02 | 724.1 | 348.80 | 3998 |
|  |  | 297.40 | 10.42 | 346.18 | 597.6 | 374.67 | 2626 |
|  |  | 306.67 | 25.27 | 352.90 | 941.6 | 368.46 | 1999 |
|  |  | 310.71 | 36.37 | 338.91 | 359.7 | 387.32 | 4398 |
|  |  | 302.92 | 17.84 | 346.85 | 629.9 | 357.44 | 1200 |
|  |  | 318.58 | 72.36 | 350.69 | 820.2 | 362.57 | 1528 |
|  |  | 282.13 | 2.10 | 349.15 | 751.1 | 353.51 | 995 |
|  |  | 277.85 | 1.30 | 341.72 | 441.7 | 353.33 | 985 |
|  |  | 288.50 | 4.21 | 348.6 | 717.3 |  |  |

TABLE 4.1.1.2.2 (Continued)

5.

| Colomina et al. 1982 |  | Grayson \& F. 1982 |  | Sonnefeld et al. 1983 |  | Van Ekeren et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| effusion |  | gas saturation |  | gas saturation-HPLC |  | spinning-rotor gauge |  |
| T/K | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | T/K | P/Pa |
| 271.46 | 0.611 | 28.9 | 16.38 | 14.15 | 3.13 | 244.19 | 0.0163 |
| 275.08 | 0.94 | 42.7 | 58.33 | 14.15 | 3.24 | 245.31 | 0.0191 |
| 277.10 | 1.19 | 50 | 100.99 | 14.15 | 3.27 | 245.31 | 0.0192 |
| 279.93 | 1.63 | 60.2 | 264.32 | 19.49 | 6.0 | 246.59 | 0.0233 |
| 281.16 | 1.99 | 69.6 | 519.1 | 19.49 | 6.19 | 247.74 | 0.0268 |
| 282.69 | 2.23 | 79 | 970.5 | 25.05 | 10.1 | 247.74 | 0.0272 |
| 283.80 | 2.54 | 20 | 6.75 | 15.05 | 10.8 | 249.18 | 0.0373 |
| 284.63 | 2.80 |  |  | 25.05 | 10.4 | 250.45 | 0.04 |
|  |  | eq. 1a | $\mathrm{P} / \mathrm{mmHg}$ | 32.1 | 20.9 | 252.77 | 0.0554 |
| $\Delta \mathrm{H}_{\text {subl }} / \mathrm{KJ} \mathrm{mol}^{\circ} 1=72.8$ |  | A | 31.80 | 32.05 | 21.0 | 255.86 | 0.0834 |
|  | at $25^{\circ} \mathrm{C}$ | B | 8753 | 32.1 | 20.8 |  |  |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\text {subl }} / \mathrm{kJ} \mathrm{mol}{ }^{\circ} 1=$ |  |
| eq. 1 | $\mathrm{P} / \mathrm{Pa}$ |  |  | eq. 1 | $\mathrm{P} / \mathrm{Pa}$ | 248.51 | 72.92 |
| A | 14.01 |  |  | A | 14.299 | 298.15 | 72.92 |
| B | 3861.80 |  |  | B | 3960.03 |  |  |

6. 

| Sato et al. 1986 |  | Sasse et al. 1988 |  |  |  | Wania et al. 1994 gas saturation-GC |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation-electrobalance |  | gas saturation |  |  |  |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | $t^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  | solid |  | liquid |  |  |  |
| 24.85 | 10.7 | -12.15 | 0.1653 | 80.16 | 968.85 | -30.6 | 0.014 |
| 28.35 | 14.9 | -12.1 | 0.1653 | 84.90 | 1240.4 | -25.0 | 0.0217 |
| 30.95 | 19.2 | -9.47 | 0.2266 | 84.93 | 1270.6 | -20.1 | 0.0586 |
| 34.15 | 25.9 | 0.52 | 0.8199 | 87.16 | 1382.6 | -14.9 | 0.108 |
| 41.65 | 52.8 | 10.17 | 2.413 | 84.23 | 1395.9 | -10.0 | 0.2122 |
| 45.35 | 71.1 | 20.11 | 7.093 | 90.15 | 1590.5 | -5.0 | 0.348 |
| 48.95 | 97.5 | 20.16 | 7.026 |  |  | 0 | 0.7634 |
| 49.45 | 101 | 29.98 | 18.265 | For liquid |  |  |  |
| 51.85 | 124 | 30.03 | 18.80 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | $\begin{gathered} \Delta \mathrm{H}_{\text {sul }} / \mathrm{kJ} \mathrm{~mol}{ }^{-1}=73.7 \\ \left(-30 \text { to } 0^{\circ} \mathrm{C}\right) \end{gathered}$ |  |
| 55.35 | 165 | 40.04 | 44.93 | A | 2.25180 |  |  |
| 57.75 | 200 | 40.04 | 45.46 | B | 76.496 |  |  |
|  |  | 50.04 | 106.8 | C | -25.09 | eq. 1 | $\mathrm{P} / \mathrm{Pa}$ |

TABLE 4.1.1.2.2 (Continued)

| Sato et al. 1986 |  | Sasse et al. 1988 |  |  |  | Wania et al. 1994 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation-electrobalance |  | gas saturation |  |  |  | gas saturation-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| eq. 3 | $\mathrm{P} / \mathrm{Pa}$ | 50.04 | 105.2 |  |  | A | 13.93 |
| A | 22.892960 .05 | 60.05 | 238.2 |  |  | B | 3851 |
| B | 4025.3560 .12 | 60.12 | 232.6 |  |  |  |  |
| C | -102.34370.11 | 70.11 | 491.0 |  |  |  |  |
|  |  | 70.16 | 491.02 |  |  |  |  |
| For solid |  |  |  |  |  |  |  |
|  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |
|  |  | A | 10.05263 |  |  |  |  |
|  |  | B | 2907.918 |  |  |  |  |
|  |  | C | 236.459 |  |  |  |  |



FIGURE 4.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for naphthalene.
TABLE 4.1.1.2.3
Reported Henry's law constants of naphthalene at various temperatures
Alaee et al. 1996

| gas stripping-GC |  |
| :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m} \mathbf{~ m}^{3} \mathbf{m o l}\right)$ |
| 3.7 | 9.65 |
| 9.4 | 15.4 |
| 15.3 | 21.4 |
| 15.5 | 23.1 |
| 20 | 33.2 |
| 25 | 42.6 |
| 25.4 | 45.2 |
| 30.2 | 58.6 |

(Continued)

TABLE 4.1.1.2.3 (Continued)

| Alaee et al. 1996 |  |
| :--- | :---: |
| gas stripping-GC |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C}$ | $\mathbf{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ |
| 35.5 | 79.1 |
| enthalpy of volatilization: |  |
| $\Delta \mathrm{H}_{\mathrm{vol}} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=44.6$ at $20^{\circ} \mathrm{C}$ |  |
| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| eq. 1 | $\mathrm{~K}_{\mathrm{AW}}$ |
| A | -5364.4 |
| B | 13.95 |



FIGURE 4.1.1.2.3 Logarithm of Henry's law constant versus reciprocal temperature for naphthalene.

### 4.1.1.3 1-Methylnaphthalene



Common Name: 1-Methylnaphthalene
Synonym: $\alpha$-methylnaphthalene
Chemical Name: 1-methylnaphthalene
CAS Registry No: 90-12-0
Molecular Formula: $\mathrm{C}_{11} \mathrm{H}_{10}$
Molecular Weight: 142.197
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-30.43 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
244.7 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$1.02015,1.01649 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
1.0125 (Dean 1985)
1.0202 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$139.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
169.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
60.06, $45.48 \quad\left(25^{\circ}, \mathrm{bp}\right.$, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :

### 4.853 (Dean 1985)

4.98, 6.95; $11.92 \quad\left(-32.45,34.25^{\circ} \mathrm{C}\right.$, total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
20.69, $28.82 \quad\left(-32.45,34.25^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)
49.3, 44.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
25.8 (shake flask-GC, Eganhouse \& Calder 1976)
28.5 (shake flask-fluorescence, Mackay \& Shiu 1977)
29.9* (shake flask-fluorescence, measured range $8.6-31.7^{\circ} \mathrm{C}$, Schwarz \& Wasik 1977)
29.5* (shake flask-fluorescence, measured range $10-25^{\circ} \mathrm{C}$, Schwarz 1977)
31.7 (generator column-HPLC, Wasik et al. 1983)
27.02 (average lit. value, Pearlman et al. 1984)
$30.2^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-GC, measured range $20-70^{\circ} \mathrm{C}$, Burris \& MacIntyre 1986)
28.0 (recommended, IUPAC Solubility Data Series, Shaw 1989)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
7.165* (manometer, extrapolated-Antoine eq., Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03592-1826.948 /\left(195.002+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $142.1-254.4^{\circ} \mathrm{C}$ (Antoine eq., Hg manometer, Camin \& Rossini 1955)
8.95 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.06899-1852.674 /\left(197.716+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $130-305^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
66.66* (52.8 ${ }^{\circ} \mathrm{C}, \mathrm{Hg}$ manometer, measured range $52.8-243.0^{\circ} \mathrm{C}$, Myers \& Fenske 1955)
7.19* (interpolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03592-1826.948 /\left(195.002+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $107.68-278.32^{\circ} \mathrm{C}$ (liquid, Antoine eq., Zwolinski \& Wilhoit 1971)
8.82* (gas saturation-GC, Macknick \& Prausnitz 1979)
8.84 (extrapolated-Clapeyron eq., Macknick \& Prausnitz 1979)
$\log (\mathrm{P} / \mathrm{mmHg})=20.552-6933.2 /(\mathrm{T} / \mathrm{K})$; temp range $5.70-38.6^{\circ} \mathrm{C}$ (Clapeyron eq., gas saturation, Macknick \& Prausnitz 1979)
$7221^{*} \quad\left(151.15^{\circ} \mathrm{C}\right.$, differential pressure gauge, measured range $151.15-271.70^{\circ} \mathrm{C}$, Wieczorek \& Kobayashi 1981)
$\log (\mathrm{P} / \mathrm{atm})=[1-517.727 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.863323-5.26355 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+3.85750 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range 278.85-593.38 K (Cox eq., Chao et al. 1983)
8.84 (interpolated Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.15971-1825.586 /\left(194.848+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $142.1-245.3^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
7.43, 6.38 (GC-RT correlation with BP-1 column, Apolane column, Bidleman 1984)
7.816 (extrapolated Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03592-1826.946 /\left(195.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $108-278^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
0.895 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.03469-3006.467 /(\mathrm{T} / \mathrm{K})$; temp range $278-313 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.15928-1826.402 /(-72.779+\mathrm{T} / \mathrm{K})$; temp range $415-526 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
8.93* (pressure gauge, interpolated-Antoine eq. derived from exptl. data, temp range -14.44 to $+115^{\circ} \mathrm{C}$, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=7.27126-2006.862 /\left(212.625+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -14.44 to $115.1^{\circ} \mathrm{C}$, (Antoine eq., pressure gauge, Sasse et al. 1998)
$7.43 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with eicosane as reference standard, Hinckley et la. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=29.8895-3.9535 \times 10^{3} /(\mathrm{T} / \mathrm{K})-7.2253 \cdot \log (\mathrm{~T} / \mathrm{K})+1.1109 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+8.9552 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}$; temp range $243-722 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
8.94, 8.93; 9.50, 8.12, 19.7; 7.42, 5.93 (quoted exptl. values; calculated; GC-RT correlation, Delle Site 1997) $\log (\mathrm{P} / \mathrm{kPa})=6.39609-2006.662 /[(\mathrm{T} / \mathrm{K})-60.525]$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
6.55; 1.28 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ : calibrated GC-RT correlation, GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3258 /(\mathrm{T} / \mathrm{K})+11.74 ; \Delta \mathrm{H}_{\text {vap }}=-62.4 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
$8.85^{*} \quad\left(24.05^{\circ} \mathrm{C}\right.$, transpiration method, measured range $294.1-324.2 \mathrm{~K}$, Verevkin 2003)
$\ln \left(\mathrm{P} / \mathrm{P}^{\mathrm{o}}\right)=298.831 / \mathrm{R}-83537.555 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(78.6 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]$; where $\mathrm{P}^{\circ}=101.325 \mathrm{kPa}$, gas constant $\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}$ (vapor pressure eq. from transpiration measurements, temp range 294.1-324.2 K, Verevkin 2003)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{Cor}$ as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
26.3 (gas stripping, Mackay et al. 1979,1982)
26.3 (gas stripping-GC, Mackay et al. 1982)
62.0 (wetted-wall column-GC, Fendinger \& Glotfelty 1990)
36.5 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
24.3 (gas stripping-GC, Shiu \& Mackay 1997)
52.1 (gas stripping-GC, Altschuh et al. 1999)
47.8* (gas stripping-GC; measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-5821.5 /(\mathrm{T} / \mathrm{K})+15.636 ; \Delta \mathrm{H}=48.4 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :

| 3.87 | (shake flask-fluorometry, Krishnamurthy \& Wasik 1978) |
| :--- | :--- |
| 3.87 | (Hansch \& Leo 1979) |
| 3.87 | (recommended, Sangster 1989, 1994) |
| 3.87 | (recommended, Hansch et al. 1995) |

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.33, 3.06 (Lula aquifer $0.032 \%$ OC, Apalachee soil $1.4 \%$ OC, batch equilibrium-sorption isotherm, Stauffer \& MacIntyre 1986)
3.36 (sediment from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
2.96-3.83 (aquifer materials, Stauffer et al. 1989)

Environmental Rate Constants, $k$, or Half-Lives; $t_{1 / 2}$ :
Volatilization:
Photolysis: calculated $t_{1 / 2}=22 \mathrm{~h}$ for direct sunlight photolysis of $50 \%$ conversion at $40^{\circ} \mathrm{N}$ latitude of midday in midsummer in near surface water, $\mathrm{t}_{1 / 2}=180 \mathrm{~d}$ in 5-m deep inland water and $\mathrm{t}_{1 / 2}=190 \mathrm{~d}$ in inland water with a suspended sediment concentration of $20 \mathrm{mg} / \mathrm{L}$ partitioning (Zepp \& Schlotzhauer 1979); $\mathrm{t}_{1 / 2}=180 \mathrm{~d}$ under summer sunlight in surface water (Mill \& Mabey 1985); direct photolysis $t_{1 / 2}=11.14 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).
Oxidation: rate constant k , for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated *data at other temperatures see original reference:
$\mathrm{k}_{\mathrm{OH}}=(5.30 \pm 0.48) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{O}_{3}}<1.3 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=(3.3 \pm 0.7) \times 10^{-17}$ $\mathrm{cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson \& Aschmann 1987, 1988)
$\mathrm{k}_{\mathrm{OH}}=5.30 \times 10^{-11} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=59.77 \times 10^{-12} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}}=5.30 \times 10^{-11} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1},(4.09 \pm 0.20) \times 10^{-11} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime to be 2.9 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\cdot \mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Hydrolysis:
Biodegradation: $\mathrm{k}=0.415 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=1.7 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{t}_{1 / 2}=0.321 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.2 \mathrm{~d}$ for McLaurin sandy loam soil, all at -3.3 bar soil moisture (Park et al. 1990).
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: atmospheric lifetimes of alkyl-substituted naphthalenes due to reaction with OH radical and with $\mathrm{N}_{2} \mathrm{O}_{5}$ calculated to range from $\sim 4$ to 13 h and 20-80 d, respectively (Atkinson \& Aschmann 1987);
direct photolysis $t_{1 / 2}=11.14 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001); a calculated tropospheric lifetime to be 2.9 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\cdot \mathrm{cm}^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).
Water: computed near-surface $t_{1 / 2}=22 \mathrm{~h}$ and for direct photochemical transformation at latitude $40^{\circ} \mathrm{N}$, midday, midsummer, and $t_{1 / 2}=80 \mathrm{~d}$ with no sediment-water partitioning and $t_{1 / 2}=190 \mathrm{~d}$ with sediment-water partitioning for direct photolysis in 5 m deep inland water body integrated over full summer d at latitude $40^{\circ} \mathrm{N}$ (Zeep \& Schlotzhauer 1979);
$t_{1 / 2}=180 \mathrm{~d}$ under summer sunlight (Mill \& Mabey 1985).
Soil: biodegradation $\mathrm{k}=0.415 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=1.7 \mathrm{~d}$ for Kidman sandy loam soil, $\mathrm{k}=0.321 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=2.2 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990).
Sediment:
Biota: elimination $\mathrm{t}_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.3.1
Reported aqueous solubilities of 1-methylnaphthalene at various temperatures

| Schwarz 1977 |  | Schwarz \& Wasik 1977 |  | Burris \& MacIntyre 1986 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-fluorescence |  | shake flask-fluorescence |  | shake flask-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 8.6 | 19.91 | 10 | 22.75 | 20 | 30.2 |
| 14.5 | 22.61 | 14 | 28.44 | 70 | 87.9 |
| 17.1 | 22.89 | 20 | 28.44 |  |  |
| 20.0 | 25.31 | 25 | 29.86 |  |  |
| 23.0 | 27.59 |  |  |  |  |
| 25.0 | 30.0 |  |  |  |  |
| 26.1 | 30.43 |  |  |  |  |
| 29.2 | 33.28 |  |  |  |  |
| 31.7 | 36.26 |  |  |  |  |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=19.1$ |  |  |  |  |  |



FIGURE 4.1.1.3.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for 1-methyInaphthalene.

TABLE 4.1.1.3.2
Reported vapor pressures of 1-methyInaphthalene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| :--- | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ | $\ln \mathrm{P} / \mathrm{P}^{\mathrm{O}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]$ |  |

1. 

| Camin \& Rossini 1955 |  | Myers \& Fenske 1955 |  | Zwolinski \& Wilhoit 1971 |  | Macknick \& Prausnitz 1979 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | Hg manometer |  | selected values |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 142.140 | 5524 | 52.8 | 66.66 | 107.68 | 1333 | 5.70 | 1.760 |
| 153.600 | 8314 | 63.5 | 133.3 | 123.57 | 2666 | 11.40 | 2.920 |
| 157.539 | 9510 | 75.8 | 266.6 | 133.66 | 4000 | 18.10 | 5.248 |
| 161.689 | 10942 | 83.0 | 400.0 | 141.21 | 5333 | 22.15 | 7.133 |
| 167.212 | 13088 | 88.9 | 533.3 | 147.319 | 6666 | 28.85 | 12.59 |
| 179.971 | 19442 | 93.3 | 666.6 | 152.474 | 7999 | 32.35 | 15.73 |
| 185.505 | 22881 | 97.1 | 799.9 | 160.932 | 10666 | 34.90 | 18.93 |
| 193.280 | 28542 | 103.8 | 1067 | 167.781 | 13332 | 38.60 | 23.46 |
| 200.536 | 34832 | 108.8 | 1333 | 180.927 | 19998 |  |  |
| 208.677 | 43162 | 117.6 | 2000 | 190.846 | 26664 | eq. 1 a | $\mathrm{P} / \mathrm{mmHg}$ |
| 217.375 | 53762 | 124.4 | 2666 | 198.908 | 33331 | A | 20.552 |
| 226.498 | 67057 | 134.4 | 4000 | 205.750 | 39997 | B | 6933.2 |
| 246.243 | 84026 | 142.2 | 5333 | 217.043 | 53329 |  |  |
| 243.177 | 98081 | 148.3 | 6666 | 226.250 | 66661 |  |  |
| 243.949 | 99655 | 153.7 | 7999 | 234.084 | 79993 |  |  |
| 244.555 | 101030 | 161.9 | 10666 | 240.938 | 93326 |  |  |
| 245.326 | 102757 | 168.5 | 13332 | 242.215 | 95992 |  |  |
|  |  | 182.0 | 19998 | 243.463 | 98659 |  |  |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 191.6 | 26664 | 244.078 | 99992 |  |  |
| A | 7.03592 | 206.0 | 39997 | 244.685 | 101325 |  |  |
| B | 1826.948 | 217.0 | 53329 |  |  |  |  |
| C | 195.002 | 225.5 | 66661 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |
|  |  | 233.3 | 79993 | A | 7.03592 |  |  |
| $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=63.82$ |  | 240.0 | 93326 | B | 1826.948 |  |  |
|  | at $25^{\circ} \mathrm{C}$ | 243.0 | 101325 | C | 195.002 |  |  |
|  |  |  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 244.685 |  |  |
|  |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=46.0$ |  |  |  |  |  |
|  |  |  |  |  | at bp |  |  |

(Continued)

TABLE 4.1.1.3.2 (Continued)
2.



FIGURE 4.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for 1-methylnaphthalene.

TABLE 4.1.1.3.3
Reported Henry's law constants of 1-methylnaphthalene at various temperatures and temperature dependence equations

| Bamford et al. 1999 |  |  |
| :---: | :---: | :---: |
| gas stripping-GC/MS |  |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ |
|  |  | average |
| 4.1 | $9.41,10.7$ | 10.1 |
| 11.0 | $16.6,18.2$ | 17.4 |
| 18.0 | $27.8,30.8$ | 29.2 |
| 25.0 | $44.8,51.0$ | 47.8 |
| 31.0 | $65.7,78.2$ | 71.7 |

$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
A 15.636

B 5821.5
enthalpy, entropy change:
$\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=48.4 \pm 1.4$
$\Delta \mathrm{S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=130$
at $25^{\circ} \mathrm{C}$


FIGURE 4.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for 1-methylnaphthalene.

### 4.1.1.4 2-Methylnaphthalene



Common Name: 2-Methylnaphthalene
Synonym: $\beta$-methylnaphthalene
Chemical Name: 2-methylnaphthalene
CAS Registry No: 91-57-6
Molecular Formula: $\mathrm{C}_{11} \mathrm{H}_{10}$
Molecular Weight: 142.197
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
34.6 (Weast 1972-73; Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
241.1 (Weast 1977; Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.0058 (Weast 1982-83; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$141.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
169.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
59.40, $45.20 \quad\left(25^{\circ}\right.$, bp, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
11.924 (Parks \& Huffman 1931)
5.61, 12.13; 17.74 ( $15.35,34.25^{\circ} \mathrm{C}$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
$39.25 \quad$ (Tsonopoulos \& Prausnitz 1971)
19.43, $39.43 \quad\left(15.35,34.25^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)
58.87, 44.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.805 ( mp at $34.6^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
24.6 (shake flask-GC, Eganhouse \& Calder 1976)
25.4 (shake flask-fluorescence, Mackay \& Shiu 1977)
20.0 (Vozñáková et al. 1978)
25.6 (average lit. value, Pearlman et al. 1984)
27.3 (generator column-HPLC, Vadas et al. 1991)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
9.07* (Hg manometer, extrapolated-Antoine eq., Camin \& Rossini 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.06850-1840.268 /\left(198.395+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $139.1-242^{\circ} \mathrm{C}$ (Antoine eq., Hg manometer, Camin \& Rossini 1955)
10.67 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.06850-1840.268 /\left(198.395+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$, temp range $130-300^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
9.07* (extrapolated-Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.06850-1840.268 /\left(198.395+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $104.85-274.3^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
9.07 (extrapolated-Antoine eq., Boublik et al. 1973)
$5.60 \quad\left(20^{\circ} \mathrm{C}\right.$, Vozñáková et al. 1978)
8629* ( $151.26^{\circ} \mathrm{C}$, differential pressure gauge, measured range $151.26-279.81^{\circ} \mathrm{C}$, Wieczorek \& Kobayashi 1981)
$\log (\mathrm{P} / \mathrm{atm})=[1-514.242 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.879050-5.85793 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+4.19235 \times 10^{-7} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; temp range 378.0-629.32 K (Cox eq., Chao et al. 1983)
9.08 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.19638-1842.831 /\left(198.692+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $139.2-241.76^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
6.31 (GC-RT correlation, supercooled liquid, Bidleman 1984)
9.033 (extrapolated, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0685-1840.268 /\left(198.4+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $105-274^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
9.33 (extrapolated from Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.21475-1858.19 /(-72.479+\mathrm{T} / \mathrm{K})$; temp range $423-515 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=56.2052-5.2563 \times 10^{3} /(\mathrm{T} / \mathrm{K})-16.195 \cdot \log (\mathrm{~T} / \mathrm{K})+8.1583 \times 10^{-11} \cdot(\mathrm{~T} / \mathrm{K})+3.0253 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 308-761 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
32.23 (wetted-wall column-GC, Fendinger \& Glotfelty 1990)
50.6 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
20.265* ( $26^{\circ} \mathrm{C}$ EPICS-GC, Hansen et al. 1993)
46.0 (gas stripping-HPLC/fluo., De Maagd et al. 1998)
62.0 (gas stripping-GC, Altschuh et al. 1999)
51.3* (gas stripping-GC; Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-5099.83 /(\mathrm{T} / \mathrm{K})+13.23 ; \Delta \mathrm{H}=42.4 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$18620\left(20^{\circ} \mathrm{C}\right.$, selected value based on Hansen et al. 1993 data, Staudinger \& Roberts 1996,2001$)$
$\log \mathrm{K}_{\mathrm{AW}}=2.245-399 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.864 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
3.86 (Hansch \& Leo 1979)
4.11 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
3.70 (HPLC-k' correlation, Hanai et al. 1981)
4.01 (HPLC-RT correlation, Eadsforth 1986)
4.09 (HPLC-RT correlation, Wang et al. 1986)
4.00 (recommended, Sangster 1989)
3.86 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
2.61 (quoted from Davies \& Dobbs 1984, Sabljic 1987)
2.65 (calculated-MCI $\chi$, Sabljic 1987)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.93 (natural sediments, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
3.40 (sediment 4.02\% from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
3.719; 3.72, 3.71 (sediment: concn ratio $\mathrm{C}_{\text {sed }} / \mathrm{C}_{\mathrm{w}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter \& Alden 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: $t_{1 / 2}($ calc $)=54 \mathrm{~h}$ for direct sunlight photolysis at $40^{\circ} \mathrm{N}$ latitude of midday in midsummer in near surface water, $t_{1 / 2}=410 \mathrm{~d}$ in inland water and $t_{1 / 2}=440 \mathrm{~d}$ in inland water with sediment partitioning (Zepp \& Schlotzhauer 1979);
$\mathrm{t}_{1 / 2}=410 \mathrm{~d}$ under summer sunlight in surface water (Mill \& Mabey 1985);
$\mathrm{k}=0.042 \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=6.4 \mathrm{~h}$ in distilled water (Fukuda et al. 1988);
direct photolysis $\mathrm{t}_{1 / 2}=9.23 \mathrm{~h}$ predicted - QSPR, in atmospheric aerosol (Chen et al. 2001).
Hydrolysis:

Oxidation: rate constant, k for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(5.23 \pm 0.42) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated atmospheric lifetime of $\sim 5 \mathrm{~h}$, and $\mathrm{k}_{\mathrm{O}_{3}}<4 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate, Atkinson \& Aschmann 1986)
$\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=(4.2 \pm 0.9) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson \& Aschmann 1987)
$\mathrm{k}_{\mathrm{OH}}=5.23 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{O}_{3}}<0.4 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=4.2 \times 10^{-17} \mathrm{~cm}^{3}$ molecule $^{-1}$
$\mathrm{s}^{-1}$ with $\mathrm{N}_{2} \mathrm{O}_{5}$ at room temp. (Atkinson \& Aschmann 1987, 1988)
$\mathrm{k}_{\mathrm{OH}}=52.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1989, 1990)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=57.36 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}}=(4.86 \pm 0.25) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 2 \mathrm{~K}$ with a calculated tropospheric lifetime to be 3.4 h using a global tropospheric $12-\mathrm{h}$ daytime average OH radical concn of $2.0 \times 10^{6} \mathrm{molecule} / \mathrm{cm}^{3}$ (relative rate method, Phousongphouang \& Arey 2002)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: calculated atmospheric lifetime of $\sim 4 \mathrm{~h}$ due to reaction with OH radical (Atkinson \& Aschmann 1986)
atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radicals and with $\mathrm{N}_{2} \mathrm{O}_{5}$ can be calculated to range from $\sim 4$ to 13 h and 20-80 d, respectively (Atkinson \& Aschmann 1987); direct photolysis $\mathrm{t}_{1 / 2}=9.23 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001);
a calculated tropospheric lifetime to be 3.4 h using a global tropospheric 12-h daytime average OH radical concn of $2.0 \times 10^{6}$ molecule $/ \mathrm{cm}^{3}$ for the reaction with OH radical (Phousong-phouang \& Arey 2002).
Surface water: computed near-surface $t_{1 / 2}=54 \mathrm{~h}$ and for direct photochemical transformation at latitude $40^{\circ} \mathrm{N}$,
midday, midsummer; $t_{1 / 2}=410 \mathrm{~d}$ with no sediment-water partitioning and $t_{1 / 2}=440 \mathrm{~d}$ with sediment-water partitioning by direct photolysis in a 5-m deep Inland Water Body (Zepp \& Schlotzhauer 1979);
$t_{1 / 2}=410$ d under summer sunlight (Mill \& Mabey 1985);
rate constants and half-lives: $\mathrm{k}=0.064 \mathrm{~d}^{-1}$, $\mathrm{t}_{1 / 2}=11 \mathrm{~d}$ in spring at $8-16^{\circ} \mathrm{C}, \mathrm{k}=0.687 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=1.0 \mathrm{~d}$ in summer at $20-22^{\circ} \mathrm{C}, \mathrm{k}=0.054 \mathrm{~d}^{-1}, \mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in winter at $3-7^{\circ} \mathrm{C}$ for the periods when volatilization appears to dominate, and $\mathrm{k}=0.046 \mathrm{~d}^{-1}$, $\mathrm{t}_{1 / 2}=15.1 \mathrm{~d}$ with $\mathrm{HgCl}_{2}$ as poison, and $\mathrm{k}=0.954 \mathrm{~d}^{-1}$, $\mathrm{t}_{1 / 2}=0.7 \mathrm{~d}$ without poison in September 9-15, in marine mesocosm experiments (Wakeham et al. 1983)
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.4.1
Reported vapor pressures of 2-methylnaphthalene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+t /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$

Camin \& Rossini 1955

| ebulliometry |  | selected values |  | differential pressure gauge |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 139.193 | 5536 | 104.85 | 1333 | 151.26 | 8629 |
| 145.431 | 6951 | 120.68 | 2666 | 158.72 | 10992 |
| 150.655 | 8339 | 130.73 | 4000 | 164.34 | 13183 |

TABLE 4.1.1.4.1 (Continued)

| Camin \& Rossini 1955 |  | Zwolinski \& Wilhoit 1971 |  | Wieczorek \& Kobayashi 1981 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ebulliometry |  | selected values |  | differential pressure gauge |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa |
| 154.676 | 9539 | 138.25 | 5333 | 169.89 | 15615 |
| 158.689 | 10942 | 144.329 | 6666 | 175.93 | 18756 |
| 164.155 | 13100 | 149.459 | 7999 | 181.84 | 22550 |
| 176.722 | 19433 | 157.872 | 10666 | 189.18 | 27850 |
| 182.322 | 22882 | 164.486 | 13332 | 196.20 | 33812 |
| 190.033 | 28551 | 177.752 | 19998 | 202.04 | 39538 |
| 197.234 | 34820 | 187.610 | 26664 | 209.49 | 48007 |
| 205.329 | 43163 | 195.619 | 33331 | 217.00 | 57974 |
| 213.963 | 53782 | 202.414 | 39997 | 225.34 | 70794 |
| 223.026 | 67089 | 213.626 | 53329 | 232.47 | 83506 |
| 239.613 | 98125 | 222.764 | 66661 | 239.90 | 96992 |
| 240.336 | 99734 | 230.537 | 79993 | 246.90 | 114865 |
| 240.957 | 101114 | 237.336 | 93326 | 254.69 | 134992 |
| 241.760 | 102929 | 238.602 | 95992 | 263.24 | 160539 |
|  |  | 239.840 | 98659 | 271.29 | 188158 |
| eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 240.449 | 99992 | 279.81 | 221176 |
| A | 7.06850 | 241.052 | 101325 |  |  |
| B | 1840.268 |  |  | exptl | itted to |
| C | 198.395 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | Chebys | lynomial |
| bp/ ${ }^{\circ} \mathrm{C}$ | 241.052 | A | 7.06850 | temp ra | 4-639 K |
|  |  | B | 1840.268 |  |  |
|  |  | C | 198.395 |  |  |
|  |  | bp/ ${ }^{\circ} \mathrm{C}$ | 241.052 |  |  |
|  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ} \mathrm{mo}$ | $46.0$ |  |  |



FIGURE 4.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylnaphthalene.

## TABLE 4.1.1.4.2

Reported Henry's law constants of 2-methylnaphthalene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$



FIGURE 4.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for 2methyInaphthalene.

### 4.1.1.5 1,3-DimethyInaphthalene



Common Name: 1,3-Dimethylnaphthalene
Synonym:
Chemical Name: 1,3-dimethylnaphthalene
CAS Registry No: 575-41-7
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-6.0 (Weast 1982-83, Dean 1985; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
263 (Dreisbach 1955; Weast 1982-83; Dean 1985; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.0063,1.0026 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
1.0144 (Weast 1982-83; Dean 1985; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$154.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : 69.58, $48.69 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
8.00 (shake flask-fluorescence, Mackay \& Shiu 1977)
7.81 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
1.947 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0469-1845.6 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $150-313^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{atm})=[1-540.353 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{1.72680-7.87991 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+42.8535 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range 400.0-541.0 K (Cox eq., Chao et al. 1983)
6.950 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.6347-2295.4 /\left(232.4+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-148^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
$\log (\mathrm{P} / \mathrm{mmHg})=7.2698-2076.0 /\left(210+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $148-310^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
71.03 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.421 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
4.42 (Hansch \& Leo 1979)
4.42 (recommended, Sangster 1993)
4.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}}^{3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated *data at other temperatures see original reference:
$\mathrm{k}_{\mathrm{OH}}=(7.49 \pm 0.39) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

### 4.1.1.6 1,4-DimethyInaphthalene



Common Name: 1,4-Dimethylnaphthalene Synonym:
Chemical Name: 1,4-dimethylnaphthalene
CAS Registry No: 571-58-4
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
$7.60 \quad$ (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
268 (Dreisbach 1955, Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
1.0166, $1.0129 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
1.0166 (Weast 1982-83)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$153.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
$70.315,48.62 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1955)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
10.6 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}$ ( $\mathrm{J} / \mathrm{mol} \mathrm{K}$ ):
37.87, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}, \mathrm{F}: 1.0$

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
11.4 (shake flask-fluorescence, Mackay \& Shiu 1977)
11.40 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
1.55 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0527-1869.0 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $155-310^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{atm})=[1-544.363 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{1.57594-8.55425 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+51.4189 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range 397.0-544 K (Cox eq., Chao et al. 1983)
2.27 (calculated-TSA, Amidon \& Anik 1981; selected, Ma et al. 1990)
4.50 (interpolated, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.6347-2345.8 /\left(232.6+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-148^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992 )
$\log (\mathrm{P} / \mathrm{mmHg})=7.2698-2076.0 /\left(210+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $148-310^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
48.84 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.372 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
4.37 (Hansch \& Leo 1979)
4.37 (recommended, Sangster 1989, 1993)
4.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated $*$ data at other temperatures see original reference:
$\mathrm{k}_{\mathrm{OH}}=(5.79 \pm 0.36) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

### 4.1.1.7 1,5-DimethyInaphthalene



Common Name: 1,5-Dimethylnaphthalene Synonym:
Chemical Name: 1,5-dimethylnaphthalene
CAS Registry No: 571-61-9
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
82 (Dreisbach 1955; Weast 1982-83; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
265 (Dreisbach 1955; Weast 1982-83; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.276 (mp at $82^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
2.74 (shake flask-GC, Eganhouse \& Calder 1976)
3.38 (shake flask-fluorescence, Mackay \& Shiu 1977)
3.12 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations.):
$\log (\mathrm{P} / \mathrm{mmHg})=7.0493-1855.0 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $150-313^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1.93; 0.513 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3346 /(\mathrm{T} / \mathrm{K})+11.51 ; \Delta \mathrm{H}_{\text {vap }}=-64.1 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
35.5 (gas stripping-fluorescence, Mackay et al. 1982)
61.8 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
36.3 (gas stripping, Shiu \& Mackay 1997)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.38 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
4.38 (Hansch \& Leo 1979)
4.38 (recommended, Sangster 1989, 1993)
4.38 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated $*$ data at other temperatures see original reference: $\mathrm{k}_{\mathrm{OH}}=(6.01 \pm 0.35) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: a calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

### 4.1.1.8 2,3-DimethyInaphthalene



Common Name: 2,3-Dimethylnaphthalene
Synonym: guaiene
Chemical Name: 2,3-dimethylnaphthalene
CAS Registry No: 581-40-8
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
105 (Dreisbach 1955; Weast 1972-73; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
268 (Dreisbach 1955; Weast 1982-83; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.003 (Weast 1982-83; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$155.8 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
70.315, $48.97 \quad\left(25^{\circ} \mathrm{C}\right.$, bp, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$25.10 \quad$ (Ruelle \& Kesselring 1997)
15.9 (Chickos et al.1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
42.06, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.164 ( mp at $105^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
1.99 (shake flask-GC, Eganhouse \& Calder 1976)
3.0 (shake flask-fluorescence, Mackay \& Shiu 1977)
2.50 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
1.55 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0527-1869.0 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $155-315^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
1.86 (extrapolated-Cox eq., Chao et al. 1983)
$\log (\mathrm{P} / \mathrm{atm})=[1-631.969 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{1.09999-10.2378 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+11.3931 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; temp range 333.15-408.15 K(Cox eq., Chao et al. 1983)
0.91 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.27335-1383.083 /\left(141.333+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $105-135^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.543 (interpolated, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.40396-2111.9 /\left(201.1+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-155^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0527-1869 /\left(180+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $155-315^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
0.437 (Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.635-4172.6 /(\mathrm{T} / \mathrm{K})$; temp range 278-301 K (Antoine eq.-I, Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=8.97875-2959.733 /(-59.936+\mathrm{T} / \mathrm{K})$; temp range 333-373 K (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.18084-1544.764 /(-116.821+\mathrm{T} / \mathrm{K})$; temp range $378-408 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
38.92 (calculated-P/C, Eastcott et al. 1988)
92.16, 64.9 (quoted, calculated-bond contribution method, Meylan \& Howard 1991)
59.9 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.396 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
$4.40 \quad$ (Hansch \& Leo 1979)
4.40 (recommended, Sangster 1993)
4.40 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Hydrolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(7.68 \pm 0.48) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, with a calculated atmospheric lifetime of $\sim 4 \mathrm{~h}$, and $\mathrm{k}_{\mathrm{O}_{3}}<4 \times 10^{-19} \mathrm{~cm}^{3}$ molecule $\mathrm{s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson \& Aschmann 1986)
$\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=(5.7 \pm 1.9) \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with $\mathrm{N}_{2} \mathrm{O}_{5}$ at $298 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson \& Aschmann 1987)
$\mathrm{k}_{\mathrm{O}_{3}}<0.4 \times 10^{-18} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=7.68 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}=5.7 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ with $\mathrm{N}_{2} \mathrm{O}_{5}$ at room temp. (Atkinson \& Aschmann 1987, 1988)
$\mathrm{k}_{\mathrm{OH}}=(76.8 \pm 4.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $295 \pm 1 \mathrm{~K}$ (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=77 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (Atkinson 1990)
$\mathrm{k}_{\mathrm{OH}}=100.3 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}}=(6.15 \pm 0.47) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ using a relative rate method with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6} \mathrm{molecule} \mathrm{cm}^{-3}$ (Phousongphouang \& Arey 2002)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: calculated atmospheric lifetime of $\sim 4 \mathrm{~h}$ due to reaction with OH radical (Atkinson \& Aschmann 1986); the atmospheric lifetimes of naphthalene and alkyl-substituted naphthalenes due to reaction with OH radicals and with $\mathrm{N}_{2} \mathrm{O}_{5}$ can be calculated to range from $\sim 4$ to 13 h and $20-80 \mathrm{~d}$, respectively (Atkinson \& Aschmann 1987);
calculated tropospheric lifetime ranging from 1.9 to 2.4 h for dimethylnaphthalenes using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6} \mathrm{molecule}^{\mathrm{cm}}{ }^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).

## Surface water:

Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

### 4.1.1.9 2,6-DimethyInaphthalene



Common Name: 2,6-Dimethylnaphthalene
Synonym:
Chemical Name: 2,6-dimethylnaphthalene
CAS Registry No: 581-42-0
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
112 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
262 (Dreisbach 1955; Dean 1985; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.003, $0.999 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
1.142 (Dean 1985)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
155.8 (calculated-density)
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $69.45,48.70 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1955)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 24.27 (Tsonopoulos \& Prausnitz 1971)
25.06 (calorimetry, Osborn \& Douslin 1975; quoted, Ruelle \& Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
$63.18 \quad$ (Tsonopoulos \& Prausnitz 1971)
65.39, 45.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.140\left(\mathrm{mp}\right.$ at $112^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
1.30 (shake flask-GC, Eganhouse \& Calder 1976)
2.0 (shake flask-fluorescence, Mackay \& Shiu 1977)
1.72 (average lit. value, Pearlman et al. 1984)
0.997 (generator column-HPLC, Vadas et al. 1991)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
20.41 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0460-1841.0 /\left(180.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $150-310^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
0.75 (calculated-TSA, Amidon \& Anik 1981)
1.38 (extrapolated- Cox eq., Chao et al. 1983)
$\log (\mathrm{P} / \mathrm{atm})=[1-687.081 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{1.14901-11.9220 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+17.3468 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\}$; temp range 328.15-418.15 K (Cox eq., Chao et al. 1983)
1.41 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.19014-1325.209 /\left(139.781+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $111-145^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
2.036 (interpolated-Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.3968-2080.3 /\left(200.8+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $20-150^{\circ} \mathrm{C}$ (Antoine eq., Dean 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.0460-1841 /\left(180+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $150-310^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
0.378 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.290-3047.828 /(\mathrm{T} / \mathrm{K})$; temp range 333-368 K (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=8.45107-2512.509 /(-89.765+\mathrm{T} / \mathrm{K})$; temp range $384-418 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.18084-1320.21 /(-133.876+\mathrm{T} / \mathrm{K})$; temp range $384-418 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-6.9795-2.9488 \times 10^{3} /(\mathrm{T} / \mathrm{K})+7.4483 \cdot \log (\mathrm{~T} / \mathrm{K})-1.15821 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+4.3391 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 383-777 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
121 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.313 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
4.31 (Hansch \& Leo 1979)
4.38 (calculated-fragment const., Yalkowsky \& Valvani 1979, 1980)
4.31 (recommended, Sangster 1989, 1993)
4.31 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$ or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: rate constant in distilled water $\mathrm{k}=0.045 \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=15.5 \mathrm{~h}$ (Fukuda et al. 1988).
Hydrolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated $*$ data at other temperatures see original reference:
$\mathrm{k}_{\mathrm{OH}}=(6.65 \pm 0.35) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: a calculated tropospheric lifetime to be $1.9-2.4 \mathrm{~h}$ using a global tropospheric $12-\mathrm{h}$ daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995)

### 4.1.1.10 1-EthyInaphthalene



Common Name: 1-Ethylnaphthalene
Synonym: $\alpha$-ethylnaphthalene
Chemical Name: 1-ethylnaphthalene
CAS Registry No: 1127-76-0
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-13.9 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
258.6 (Lide 2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$1.00816,1.00446 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$, Dreisbach 1955)
1.0082 (Weast 1982-83; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$155.0 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{v}}(\mathrm{kJ} / \mathrm{mol})$ : 67.42, $46.92 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
10.7 (shake flask-fluorescence, Mackay \& Shiu 1977)
10.0* (shake flask-fluorescence, Schwarz \& Wasik 1977)
10.0* (shake flask-fluorescence, Schwarz 1977)
11.58 (generator column-HPLC, Wasik et al. 1981)
10.31 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
133.3* $\quad\left(70.0^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $70.0-258.1^{\circ} \mathrm{C}$, Stull 1947)
3.0 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=6.9599-1791.4 /\left(180.5+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $145-310^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
2.51* (extrapolated from liquid state, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=7.03159-1841.320 /\left(185.28+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $120-292^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{atm})=[1-531.480 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.923623-6.97505 \times 10^{-4} .(\mathrm{T} / \mathrm{K})+5.07450 \times 10^{-7} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; temp range 393.15-565.45 K (Cox eq., Chao et al. 1983)
2.51 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.15645-1841.32 /(-87.87+\mathrm{T} / \mathrm{K})$; temp range $393-565 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=7.5650-3.7597 \times 10^{3} /(\mathrm{T} / \mathrm{K})+2.6035 \cdot \log (\mathrm{~T} / \mathrm{K})-1.1581 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+5.1365 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $259-776 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
14.8 (calculated-P/C, Eastcott et al. 1988)
36.7 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
69.4 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.39 (calculated-fragment const., Yalkowsky \& Valvani 1979, 1980)
4.38 (calculated-fragment const., Yalkowsky et al. 1983)
4.42 (calculated-solvatochromic parameters and $\mathrm{V}_{\mathrm{I}}$, Kamlet et al. 1988)
$4.40 \quad$ (recommended, Sangster 1989, 1994)
4.44 (calculated-molar volume, Wang et al. 1992)
4.8016 (calculated-UNIFAC group contribution, Chen et al. 1993)
4.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.77 (sediment, HPLC-k' correlation, Vowles \& Mantoura 1987)
3.89 (HPLC-capacity factor correlation, Hodson \& Williams 1988)
3.78 (calculated-MCI ${ }^{1} \chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated *data at other temperatures see original reference:
$\mathrm{k}_{\mathrm{OH}}=(3.64 \pm 0.41) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime to be 3.8 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: a calculated tropospheric lifetime to be 3.8 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ for the reaction with OH radical (Phousongphouang \& Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.10.1
Reported aqueous solubilities and vapor pressures of 1-ethylnaphthalene at various temperatures

| Aqueous solubility |  |  |  | Vapor pressure |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Schwarz 1977 |  | Schwarz \& Wasik 1977 |  | Stull 1947 |  | Zwolinski \& Wilhoit 1971 |  |
| shake flask-fluorescence |  | shake flask-fluorescence |  | summary of literature data |  | selected values |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathbf{t}^{\circ} \mathrm{C}$ | P/Pa | $t^{\prime}{ }^{\circ} \mathrm{C}$ | P/Pa |
| 8.6 | 8.124 | 10 | 8.1 | 70.0 | 133.3 | 120.0 | 1333 |
| 11.1 | 8.124 | 14 | 8.1 | 101.4 | 666.6 | 136.04 | 2666 |
| 14.0 | 8.28 | 20 | 10 | 116.8 | 1333 | 146.22 | 4000 |
| 17.1 | 8.593 | 25 | 10 | 133.8 | 2666 | 153.85 | 5333 |
| 20.0 | 8.436 |  |  | 152.0 | 5333 | 160.01 | 6666 |
| 23.0 | 8.593 |  |  | 164.1 | 7999 | 165.22 | 7999 |
| 25.0 | 10.0 |  |  | 180.0 | 13332 | 173.76 | 10666 |
| 26.1 | 9.842 |  |  | 204.6 | 26664 | 180.67 | 13332 |
| 31.7 | 11.72 |  |  | 230.8 | 53329 | 193.94 | 19998 |
|  |  |  |  | 258.1 | 101325 | 203.96 | 26664 |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=14.27$ |  |  |  |  |  |  | $33331$ |
|  |  |  |  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | -27 | $219.01$ | 39997 |
|  |  |  |  |  |  | 230.41 | 53329 |
|  |  |  |  |  |  | 239.71 | 66661 |
|  |  |  |  |  |  | 247.62 | 79993 |
|  |  |  |  |  |  | 254.54 | 93326 |
|  |  |  |  |  |  | 255.83 | 95992 |
|  |  |  |  |  |  | 257.09 | 98659 |
|  |  |  |  |  |  | 258.94 | 101325 |
|  |  |  |  |  |  | $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
|  |  |  |  |  |  |  | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  |  |  |  |  | A | 7.03159 |
|  |  |  |  |  |  | B | 1841.320 |
|  |  |  |  |  |  | C | 185.28 |
|  |  |  |  |  |  | $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 258.33 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}} /\left(\mathrm{kJ} \mathrm{~mol}^{-}\right.$ |  |
|  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ | - |
|  |  |  |  |  |  | at bp | 48.1 |



FIGURE 4.1.1.10.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 1-ethyInaphthalene.


FIGURE 4.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-ethylnaphthalene.

### 4.1.1.11 2-EthyInaphthalene



Common Name: 2-Ethylnaphthalene
Synonym: $\beta$-ethylnaphthalene
Chemical Name: 2-ethylnaphthalene
CAS Registry No: 939-27-5
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{12}$
Molecular Weight: 156.223
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-7.4 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
258 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
0.9922 (Weast 1982-83; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$157.4 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated from density)
192.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
66.99, $47.33 \quad\left(25^{\circ}, \mathrm{bp}\right.$, Dreisbach 1955)
64.7 (Lei et al. 2002)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ ), F: 1.0
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
7.97 (shake flask-GC, Eganhouse \& Calder 1976)
7.97 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
3.76 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=8.0819-1886.0 /\left(191.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $145-300^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
3.24* (extrapolated from liq. state, Antoine eq., Zwolinski \& Wilhoit 1971; quoted, Mackay \& Shiu 1981) $\log (\mathrm{P} / \mathrm{mmHg})=7.07566-1880.73 /\left(191.41+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $119.14-291.9^{\circ} \mathrm{C}$ (Antoine eq., Zwolinski \& Wilhoit 1971)
4.21* (extrapolated exptl. data, Macknick \& Prausnitz 1979; quoted, Mackay \& Shiu 1981)
$\log (\mathrm{P} / \mathrm{mmHg})=21.485-7435.9 /(\mathrm{T} / \mathrm{K})$; temp range $13.05-45.1^{\circ} \mathrm{C}$ (Clapeyron eq., gas saturation, Macknick \& Prausnitz 1979)
$\log (\mathrm{P} / \mathrm{atm})=[1-531.189 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.871612-5.23140 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+3.70623 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range 286.2-565.05 K (Cox eq., Chao et al. 1983)
4.21 (interpolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.46683-3232.791 /(\mathrm{T} / \mathrm{K})$; temp range $286-319 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.20056-1880.73 /(-82.74+\mathrm{T} / \mathrm{K})$; temp range 393-565 K (Antoine eq.-II, Stephenson \& Malanowski 1987)
3.71* (pressure gauge in vacuum cell, interpolated-Antoine eq. derived from exptl. data, temp range, $-4.65-125^{\circ} \mathrm{C}$, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=6.83511-1799.779 /\left(189.505+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range -4.65 to $125.09^{\circ} \mathrm{C}$ (Antoine eq., pressure gauge, Sasse et al. 1988)
$\log (\mathrm{P} / \mathrm{kPa})=7.46683-3232.79 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000) 2.56; 0.633 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3381 /(\mathrm{T} / \mathrm{K})+11.75 ; \Delta \mathrm{H}_{\text {vap }}=-64.7 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
82.2 (calculated-P/C, Mackay \& Shiu 1981)
63.2 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
54.5 (gas stripping-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.377 (shake flask-fluorometry, Krishnamurthy \& Wasik 1978)
4.43 (HPLC- $\mathrm{k}^{\prime}$ correlation, Vowles \& Mantoura 1987)
4.38 (recommended, Sangster 1989, 1994)
4.38 (recommended, Hansch et al. 1995)
4.00 (HPLC-k' correlation, Ritter et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.76 (sediment $4.02 \%$ OC from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
3.76 (calculated-MCI ${ }^{1} \chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: $\mathrm{k}=0.038 \mathrm{~h}^{-1}$ in distilled water with $\mathrm{t}_{1 / 2}=18.4 \mathrm{~h}$ (Fukuda et al. 1988).
Hydrolysis:
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated *data at other temperatures see original reference: $\mathrm{k}_{\mathrm{OH}}=(4.02 \pm 0.55) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $(298 \pm 2) \mathrm{K}$ with a calculated tropospheric lifetime to be
3.5 h using a global tropospheric 12-h daytime average OH radical concentration of $2.0 \times 10^{6}$ molecule $\mathrm{cm}^{-3}$ (relative rate method, Phousongphouang \& Arey 2002)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:

Half-Lives in the Environment:
Air:
Surface water: $\mathrm{t}_{1 / 2}=18.4 \mathrm{~h}$ in distilled water (Fukuda et al. 1988).
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

TABLE 4.1.1.11.1
Reported vapor pressures of 2-ethylnaphthalene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | (1) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| :--- | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | (2) | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | (3) |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K}) \quad$ (4)
Zwolinski \& Wilhoit 1971 Macknick \& Prausnitz 1979 Sasse et al. 1988

| selected values |  | gas saturation |  | electronic manometer |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 119.14 | 1333 | 13.05 | 1.533 | -4.65 | 0.164 |
| 135.28 | 2666 | 17.90 | 2.213 | 0.26 | 0.30 |

TABLE 4.1.1.11.1 (Continued)



FIGURE 4.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for 2-ethylnaphthalene.

### 4.1.1.12 1,4,5-TrimethyInaphthalene



Common Name: 1,4,5-Trimethylnaphthalene Synonym:
Chemical Name: 1,4,5-trimethylnaphthalene
CAS Registry No: 2131-41-1
Molecular Formula: $\mathrm{C}_{13} \mathrm{H}_{14}$
Molecular Weight: 170.250
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
63 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
285 (Zwolinski \& Wilhoit 1971)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
169.0 (calculated-density, liquid molar volume, Lande \& Banerjee 1981)
214.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.424 (mp at $63^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
2.10 (shake flask-fluorescence, Mackay \& Shiu 1977)
2.04 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
0.681 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, Chao et al. 1983)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{atm}\right)=[1-558.187 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.998467-7.03095 \times 10^{-4} .(\mathrm{T} / \mathrm{K})+1.71801 \times 10^{-7} .(\mathrm{T} / \mathrm{K})^{2}\right\}$; temp range 415.15-558.15 K (Cox eq., Chao et al. 1983)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
23.50 (calculated-P/C, Eastcott et al. 1988)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.90 (calculated-fragment const., Yalkowsky \& Valvani 1979, 1980)
4.79 (calculated-solubility and mp, Mackay et al. 1980)
4.94 (calculated-solvatochromic parameters and intrinsic molar volume $\mathrm{V}_{\mathrm{I}}$, Kamlet et al. 1988)
$5.10 \pm 0.50$ (recommended, Sangster 1989)
4.91 (calculated-molar volume, Wang et al. 1992)
5.6829 (calculated-UNIFAC group contribution, Chen et al. 1993)
4.79 (recommended, Sangster 1993)
4.90 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).

### 4.1.1.13 Biphenyl



Common Name: Biphenyl
Synonym: diphenyl, phenylbenzene
Chemical Name: biphenyl
CAS Registry No: 92-52-4
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{10}$
Molecular Weight: 154.207
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
68.93 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
256.1 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.866 (Weast 1982-1983)
1.04 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$148.3 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
184.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
18.58 (Parks \& Huffman 1931) 18.66 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 51.05 (Miller et al. 1984) 54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.371\left(\mathrm{mp}\right.$ at $68.93^{\circ} \mathrm{C}$ ) 0.35 (Mackay et al. 1980, 1983; Shiu \& Mackay 1986; Shiu et al. 1987) 0.381 (calculated, $\Delta \mathrm{S}_{\text {fus }}=54 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
5.94 (shake flask-UV, Andrews \& Keefer 1949)
7.48* (shake flask-UV, measured range $0.4-42.8^{\circ} \mathrm{C}$, Bohon \& Claussen 1951)
3.87 (shake flask-UV, Sahyun 1966)
7.08* (shake flask-UV, measured range $0-64.5^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-4520 /(\mathrm{T} / \mathrm{K})+4.08 \times 10^{-4} \cdot[(\mathrm{~T} / \mathrm{K})-298.15]^{2}-20.8+0.0273 \cdot(\mathrm{~T} / \mathrm{K})$, temp range $24.6-73.4^{\circ} \mathrm{C}$
(shake flask-UV measurements, Wauchope \& Getzen 1972)
7.45 (shake flask-GC, Eganhouse \& Calder 1976)
7.0 (shake flask-fluorescence, Mackay \& Shiu 1977)
8.50 (shake flask-nephelometry, Hollifield 1979)
7.51 (shake flask-LSC, Banerjee et al. 1980)
8.09 (TLC-RT correlation, Bruggeman et al. 1982)
6.71 (generator column-GC/ECD, Miller et al. 1984, 1985; quoted, Hawker 1989b)
7.09 (recommended, Pearlman et al. 1984)
7.05 (vapor saturation-UV, Akiyoshi et al. 1987)
$6.5 \quad\left(29^{\circ} \mathrm{C}\right.$, shake flask-GC/FID; Stucki \& Alexander 1987)
7.20, 7.55 (generator column-HPLC/UV, Billington et al. 1988)
10.67 (calculated average of HPLC-RI, Brodsky \& Ballschmiter 1988)
7.2* (recommended, IUPAC Solubility Data Series, Shaw 1989)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=1.872-973.4 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=-1.5792-3669.26 /(\mathrm{T} / \mathrm{K})$, temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
5.37, 5.32 (generator column-GC/ECD, different flow rates, Oleszek-Kudlak et al. 2004)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
7933* $\quad\left(162.5^{\circ} \mathrm{C}\right.$, isoteniscope-manometer, measured range $162.5-255.2^{\circ} \mathrm{C}$, Chipman \& Peltier 1929)
$104^{*} \quad\left(69.20^{\circ} \mathrm{C}\right.$, temp range $69.20-271.2^{\circ} \mathrm{C}$, Cunningham 1930; quoted, Boublik et al. 1984)
$133.3^{*} \quad\left(70.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $70.6-254.0^{\circ} \mathrm{C}$, Stull 1947)
1.30 (effusion method, Bright 1951)
$\log (\mathrm{P} / \mathrm{mmHg})=10.38-3799 /(\mathrm{T} / \mathrm{K})$; temp range $4.0-34.5^{\circ} \mathrm{C}$ (Antoine eq., effusion, Bright 1951)
0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)
1.273* (effusion method, Bradley \& Cleasby 1953; selected, Bidleman 1984; Neely 1983; Erickson 1986)
$\log (\mathrm{P} / \mathrm{cmHg})=11.282-4263 /(\mathrm{T} / \mathrm{K})$; temp range $15.05-40.55^{\circ} \mathrm{C}$ (Antoine eq., Bradley \& Cleasby 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 12910.0 /(\mathrm{T} / \mathrm{K})]+8.218583$; temp range $70.6-254.9^{\circ} \mathrm{C}$ (Antoine eq., Weast 1972-73)
7.60 (selected $\mathrm{P}_{\mathrm{L}}$, Mackay \& Wolkoff 1973; Mackay \& Leinonen 1975; Mackay et al. 1982; Bopp 1983)
$1.41^{*}$ (effusion method, interpolated-Antoine eq., measured range 24.9-50.33 ${ }^{\circ} \mathrm{C}$, Radchenko \& Kitiagorodskii 1974; selected, Bidleman 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=12.6789-4367.436 /(\mathrm{T} / \mathrm{K})$; temp range $24.9-50.33^{\circ} \mathrm{C}$ (Antoine eq., Knudsen effusion, Radchenko \& Kitiagorodskii 1974)
$16.0^{*} \quad\left(53.05^{\circ} \mathrm{C}\right.$, gas saturation-GC, measured range 53.05-81.05${ }^{\circ} \mathrm{C}$, Sharma \& Palmer 1974)
$2040^{*} \quad\left(123.0^{\circ} \mathrm{C}\right.$, pressure transducer, measured range $123.0-327.55^{\circ} \mathrm{C}$, Nasir et al. 1980)
1.40 (HPLC-RT correlation, Swann et al. 1983)
$\log (\mathrm{P} / \mathrm{atm})=[1-528.437 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.821410-2.73337 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+1.02285 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range $:$ 342.35-673.15 K (Cox eq., Chao et al. 1983)
$5.608 \quad\left(\mathrm{P}_{\mathrm{L}}\right.$ supercooled liquid converted from literature $\mathrm{P}_{\mathrm{S}}$ with $\Delta \mathrm{S}_{\text {fus }}$ Bidleman 1984)
$3.35,3.41$ ( $\mathrm{P}_{\mathrm{GC}}$ by GC-RT correlation with octadecane as reference standard, different columns, BP-1 column, Apolane-87 column, Bidleman 1984)
$\log (\mathrm{P} / \mathrm{kPa})=6.36895-1997.558 /\left(202.608+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $69.2-271.1^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$1.19 \pm 0.03 ; 1.03,1.29,0.579,0.969$ (gas saturation-GC; quoted lit. values Burkhard et al. 1984, 1985b)
$1.15^{*} \quad\left(24.7^{\circ} \mathrm{C}\right.$, gas saturation-GC/FID, measured range $5.2-24.7^{\circ} \mathrm{C}$, Burkhard et al. 1984)
$\log (\mathrm{P} / \mathrm{Pa})=14.840-4402.1 /(\mathrm{T} / \mathrm{K})$; temp range $5.2-24.7^{\circ} \mathrm{C}$ (gas saturation data, Clapeyron eq., Burkhard et al. 1984)
$0.423,0.703,0.594$ (calculated-MW, GC-RI correlation, calculated-MCI $\chi$, Burkhard et al. 1985a)
2.03 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, GC-RI correlation, Burkhard et al. 1985b)
$\log (\mathrm{P} / \mathrm{mmHg})=7.24541-1998.725 /\left(202.733+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $69-271^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
5.61; 6.62 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, quoted lit.; GC-RT correlation, Foreman \& Bidleman 1985)
2.43; 6.90 (selected $P_{S}$; supercooled liq. $\mathrm{P}_{\mathrm{L}}$, Shiu \& Mackay 1986; Shiu et al. 1987; Sklarew \& Girvin 1987)
1.443; 1.23 ( $\mathrm{P}_{\mathrm{S}}$, interpolated - Antoine equations; Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.71929-4143.054 /(\mathrm{T} / \mathrm{K})$; temp range 297-324 K (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{S} / \mathrm{kPa}\right)=28.5175-21141.5 /(374.85+\mathrm{T} / \mathrm{K})$; temp range $283-342 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.37526-1794.8 /(-74.85+\mathrm{T} / \mathrm{K})$; temp range $390-563 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
3.35 ( $\mathrm{P}_{\mathrm{GC}}$ by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=53.0479-5.3509 \times 10^{3} /(\mathrm{T} / \mathrm{K})-14.955 \cdot \log (\mathrm{~T} / \mathrm{K})+2.1039 \times 10^{-9} \cdot(\mathrm{~T} / \mathrm{K})+2.4345 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $342-789 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
0.422-2.54; 2.03-7.04 (quoted range of lit. $\mathrm{P}_{\mathrm{S}}$ values; lit. $\mathrm{P}_{\mathrm{L}}$ values, Delle Site 1997)
5.31; 2.02 (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.05-3201 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=8.20-2228 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{kPa})=14.840-4402.1 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000) 3.63; 0.822 (supercooled liquid $P_{L}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3265 /(\mathrm{T} / \mathrm{K})+11.51 ; \Delta \mathrm{H}_{\text {vap }} .=-62.5 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):

| 41.34 | (gas stripping-GC, Mackay et al. 1979) |
| :--- | :--- |
| 30.4 | (gas stripping-GC, Mackay et al. 1980) |
| 11.55 | (gas stripping-GC, Warner et al. 1987) |
| 19.57 | (wetted-wall column-GC, Fendinger \& Glotfelty 1990) |
| 86.5 | (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991) |
| 31.20 | (gas stripping-GC, Shiu \& Mackay 1997) |
| $\log [\mathrm{H} /(\mathrm{Pa} \mathrm{m}$ |  |
|  | $3 / \mathrm{mol})]=6.33-1255 /(\mathrm{T} / \mathrm{K})$ (Passivirta et al. 1999) |

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
3.16 (shake flask-UV, Rogers \& Cammarata 1969)
4.09 (shake flask, Leo et al. 1971; Hansch \& Leo 1979)
4.04 (shake flask, Hansch et al. 1973)
4.17, 4.09, 3.16, 4.04 (Neely et al. 1974; Hansch \& Leo 1979)
3.95 (HPLC-k' correlation, Rekker \& De Kort 1979)
3.75 (HPLC-RT correlation, Veith et al. 1979a)
4.04 (shake flask-HPLC, Banerjee et al. 1980)
3.88 (lit. average, Kenaga \& Goring 1980; Freitag et al. 1985)
4.10 (RP-TLC-k' correlation, Bruggeman et al. 1982)
4.08 (HPLC-k' correlation, Hammers et al. 1982)
3.70 (HPLC-RT correlation, Woodburn 1982; Woodburn et al, 1984)
3.16-4.09, 3.91 (shake flask, range, average, Eadsforth \& Moser, 1983)
3.91-4.15, 4.05 (HPLC, range, average, Eadsforth \& Moser 1983)
4.03 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
3.93 (HPLC correlation; Harnisch et al. 1983)
3.76 (generator column-GC/ECD, Miller et al. 1984,1985)
3.89 (generator column-HPLC, Woodburn et al. 1984)
3.79 (RP-HPLC-RT correlation, Rapaport \& Eisenreich 1984)
4.11-4.13 (HPLC-RV correlation, quoted exptl., Garst 1984)
4.10 (HPLC-RV correlation, Garst \& Wilson 1984)
4.05 (HPLC-RT correlation, Edsforth 1986)
3.81 (shake flask-GC, Menges \& Armstrong 1991)
4.13 (HPLC-RT correlation, Wang et al. 1986)
3.63 (HPLC-k' correlation, De Kock \& Lord 1987)
3.89 (generator column-GC, Doucette \& Andren 1987, 1988)
4.14, 4.06, 4.00, 3.94 (RP-HPLC-RI correlation, Brodsky \& Ballschmiter 1988)
3.69 (HPLC-RT correlation, Doucette \& Andren 1988)
3.75 (HPLC-RT correlation, Sherblom \& Eganhouse 1988)
4.008; 4.10 (slow stirring-GC; calculated- $\pi$ const., De Bruijn et al. 1989; De Bruijn \& Hermens 1990)
3.98 (recommended, Sangster 1989, 1993)
4.29 (dual-mode centrifugal partition chromatography, Gluck \& Martin 1990)
4.26 (HPLC-k' correlation, Noegrohati \& Hammers 1992)
4.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
6.92, 6.09; 6.09
( $0,20^{\circ} \mathrm{C}$, multi-column GC-k' correlation; calculated at $20^{\circ} \mathrm{C}$, Zhang et al. 1999)
6.15
(calculated- $\mathrm{S}_{\text {oct }}$ and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:

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2.64 (trout, calculated-\mp@subsup{k}{1}{}/\mp@subsup{\textrm{k}}{2}{}}\mathrm{ , Neely et al. 1974)
3.12 (rainbow trout, Veith et al. 1979; Veith & Kosian 1983)
2.53 (fish, flowing water, Kenaga & Goring 1980; Kenaga 1980)
2.73, 2.45, 3.41 (algae, fish, activated sludge, Freitag et al. 1985; selected, Halfon & Reggiani 1986)
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Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.15 (soil, Kenaga 1980)
3.0, 3.27 (Aldrich humic acid, reversed phase separation, Landrum et al. 1984)
3.57, 3.77 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with $9.6 \mathrm{mg} / \mathrm{L}$ DOC: Landrum et al. 1984)
5.58, 4.04 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 $\mathrm{mg} / \mathrm{L}$ DOC, Landrum et al. 1984)
5.68, 5.34, 5.23, 3.57 (humic materials in natural water: Huron River $6.7 \%$ DOC spring, Grand River $10.7 \%$ DOC spring, Lake Michigan $4.7 \%$ DOC spring, Lake Erie $9.6 \%$ DOC spring, RP-HPLC separation method, Landrum et al. 1984)
3.52, 2.94 (Apison soil $0.11 \%$ OC, Dormont soil $1.2 \%$ OC, batch equilibrium, Southworth \& Keller 1986)
3.40 (calculated, soil, Chou \& Griffin 1987)
3.04, $3.32,3.26,3.04,3.08$ ( 5 soils: clay loam/kaolinite, light clay/montmorillonite, light clay/montmorillite, sandy loam/allophane, clay loam/allophane, batch equilibrium-sorption isotherm, Kishi et al. 1990)
4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
3.03, 3.12 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%$, $\mathrm{OC} \geq 0.5 \%$, average values, Delle Site 2001)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{P}}$ :
2.146 (lake sediment, calculated- $\mathrm{K}_{\mathrm{OW}}, \mathrm{f}_{\mathrm{OC}}$, Formica et al. 1988)

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1 / 2}$ :
Volatilization/Evaporation: $t_{1 / 2}=7.52 \mathrm{~d}$ evaporation from water depth of 1 m (Mackay \& Leinonen 1975), rate of volatilization $\mathrm{k}=0.92 \mathrm{~g} \mathrm{~m}^{-2} \mathrm{~h}^{-1}$ (Metcalfe et al. 1988)
Photolysis: $\mathrm{k}=5.1 \times 10^{-4} \mathrm{~h}^{-1}$ to $7.4 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{H}_{2} \mathrm{O}_{2}$ under photolysis at $25^{\circ} \mathrm{C}$ in $\mathrm{F}-113$ solution and with HO- in the gas (Dilling et al. 1988);
photodegradation $\mathrm{k}=5.1 \times 10^{-4} \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=22.61 \mathrm{~h}$ in methanol-water ( $3: 7, \mathrm{v} / \mathrm{v}$ ) with initial concentration of 16.2 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991).
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures see reference:
$\mathrm{k}_{\mathrm{OH}}=(8.06 \pm 0.77) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with an estimated lifetime of $\sim 3 \mathrm{~d}$, and $\mathrm{k}_{\mathrm{O}_{3}}<2.0 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $294 \pm 1 \mathrm{~K}$ (relative rate method, Atkinson et al. 1984)
$\mathrm{k}_{\mathrm{OH}}=(8.5 \pm 0.8) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 295 K (relative rate method, Atkinson \& Aschmann 1985)
$\mathrm{k}_{\mathrm{OH}}=(7 \pm 2) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1985)
$\mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=7.9 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.(5.8-8.2) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
$\mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=7.1 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{obs})=.7.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (SAR structure-activity relationship, Atkinson 1987b)
$\mathrm{k}_{\mathrm{O}_{3}}<2 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{OH}}=7.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1} ; \mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}}<2.0 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1}$ $\mathrm{s}^{-1}$ for reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ at room temp. (Atkinson \& Aschmann 1988)
$\mathrm{k}_{\mathrm{OH}} *=7.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (recommended, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=6.44 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1993)
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=7.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}($ calc $)=6.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated tropospheric lifetime of 2.0 d (Kwok et al. 1995)
Hydrolysis:
Biodegradation: $100 \%$ degraded by activated sludge in 47 h cycle (Monsanto Co. 1972);
$\mathrm{k}=109 \mathrm{yr}^{-1}$ in the water column and $\mathrm{k}=1090 \mathrm{yr}^{-1}$ in the sediment, microbial degradation pseudo firstorder rate constant (Wong \& Kaiser 1975; selected, Neely 1981);
$\mathrm{k}=9.3-9.8 \mathrm{nmol} \mathrm{L} \mathrm{L}^{-1} \mathrm{~d}^{-1}$ with an initial biphenyl concentration of $4.4-4.7 \mu \mathrm{~mol} / \mathrm{L}$, and $\mathrm{k}=3.2 \mathrm{nmol} \mathrm{L}^{-1}$ $\mathrm{d}^{-1}$ with initial concentration of $2.9 \mu \mathrm{~mol} / \mathrm{L}$, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
$\mathrm{t}_{1 / 2}=1.5 \mathrm{~d}$, estimated by using water die-away test (Bailey et al. 1983)
$t_{1 / 2}($ aq. aerobic $)=36-168 \mathrm{~h}$, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
$\mathrm{t}_{1 / 2}($ aq. anaerobic $)=144-672 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
removal rate of 5.3 and 0.52 mg ( g of volatile suspended solid d$)^{-1}$, degradation by bacteria from creosotecontaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic conditions in a fluidized bed reactor (Rockne \& Strand 1998)
Biotransformation
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants or Half-Lives:
$\mathrm{k}_{1}=6.79 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0155 \mathrm{~h}^{-1}$ (trout muscle, Neely et al. 1974; Neely 1979)
$\mathrm{k}_{1}=6.8 \mathrm{~h}^{-1} ; 1 / \mathrm{k}_{2}=65 \mathrm{~h}$ (trout, quoted, Hawker \& Connell 1985)
$\log \mathrm{k}_{1}=2.21 \mathrm{~d}^{-1} ; \log 1 / \mathrm{k}_{2}=0.43 \mathrm{~d}$ (fish, Connell \& Hawker 1988)
$\log \mathrm{k}_{2}=-0.43 \mathrm{~d}^{-1}$ (fish, quoted, Thomann 1989)
Half-Lives in the Environment:
Air: calculated lifetime of $\sim 3 \mathrm{~d}$ due to reaction with OH radical, assuming an average daytime atmospheric OH radical concn of $\sim 1 \times 10^{6}$ molecule $/ \mathrm{cm}^{3}$ (Atkinson et al. 1984);
estimated atmospheric lifetime of $\sim 2.7 \mathrm{~d}$ due to reaction with the OH radical for a 24 -h average OH radical concn of $5 \times 10^{5} \mathrm{~cm}^{-3}$ (Atkinson \& Aschmann 1985);
calculated tropospheric lifetime of 9 d due to the rate constants of gas-phase reaction with OH radical (Atkinson 1987);
$\mathrm{t}_{1 / 2}=7.8-110 \mathrm{~h}$, based on photooxidation half-life in air (Howard et al. 1991);
tropospheric lifetime of 2.0 d based on the experimentally determined rate constant for gas phase reaction with OH radical for biphenyl (Kwok et al. 1995).
Surface water: $\mathrm{t}_{1 / 2} \sim 1.5 \mathrm{~d}$ in river water (Bailey et al. 1983);
$\mathrm{t}_{1 / 2}=36-168 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
photolysis $\mathrm{t}_{1 / 2}=19.18 \mathrm{~min}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater: $\mathrm{t}_{1 / 2}=72-336 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Sediment:
Soil: $t_{1 / 2}=36-168 \mathrm{~h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biota: estimated $\mathrm{t}_{1 / 2}=29 \mathrm{~h}$ from fish in simulated ecosystem (Neely 1980).

TABLE 4.1.1.13.1
Reported aqueous solubilities of biphenyl at various temperatures

| Bohon \& Claussen 1951 |  | Wauchope \& Getzen 1972 |  |  |  | Shaw 1989 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-UV |  |  |  | IUPAC recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  |  |  | experimental |  | smoothed |  |  |
| 0.40 | 2.83 | 24.6 | 7.13 | 0 | 2.64 | 0 | 2.72 |
| 2.4 | 2.97 | 24.6 | 7.29 | 24.6 | 6.96 | 10 | 4.1 |
| 5.2 | 3.38 | 24.6 | 7.35 | 25 | 7.08 | 20 | 6.3 |
| 7.6 | 3.64 | 29.9 | 8.77 | 29.9 | 8.73 | 25 | 7.2 |
| 10 | 4.06 | 29.9 | 8.64 | 30.3 | 8.88 | 30 | 9.1 |
| 12.6 | 4.58 | 29.9 | 8.95 | 38.4 | 12.7 | 40 | 14.4 |
| 14.9 | 5.11 | 30.3 | 8.55 | 40.1 | 13.8 | 50 | 22 |
| 15.9 | 5.27 | 30.3 | 8.54 | 47.5 | 19.5 | 69 | 37 |
| 25 | 7.48 | 30.3 | 8.48 | 50 | 22.0 |  |  |
| 25.6 | 7.78 | 38.4 | 13.2 | 50.1 | 22.1 |  |  |
| 30.1 | 9.64 | 38.4 | 13.3 | 50.2 | 22.2 |  |  |
| 30.4 | 9.58 | 38.4 | 13.5 | 54.7 | 27.7 |  |  |
| 33.3 | 11.0 | 40.1 | 13.1 | 59.2 | 34.8 |  |  |
| 34.9 | 11.9 | 40.1 | 13.4 | 60.5 | 37.2 |  |  |
| 36 | 12.5 | 40.1 | 13.4 | 64.5 | 45.9 |  |  |
| 42.8 | 17.2 | 47.5 | 18.8 |  |  |  |  |

(Continued)

TABLE 4.1.1.13.1 (Continued)

| Bohon \& Claussen 1951 |  | Wauchope \& Getzen 1972 |  |  |  | Shaw 1989 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  | shake flask-UV |  |  |  | IUPAC recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | S/g.m $\mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  |  | 47.5 | 19.0 | temp | dence eq. 1 |  |  |
| for supercooled liquid: |  | 47.5 | 18.7 | $\ln x$ | mole fraction |  |  |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  | 50.1 | 20.6 | $\Delta \mathrm{H}_{\text {fus }}$ | $18.9 \pm 0.50$ |  |  |
| at 275 K | 7.03 | 50.1 | 21.6 | $10^{2} \cdot \mathrm{~b}$ | $2.73 \pm 0.12$ |  |  |
| 280 K | 10.13 | 50.1 | 21.8 | c | $20.8 \pm 0.4$ |  |  |
| 285 K | 11.25 | 50.2 | 20.7 |  |  |  |  |
| 290 K | 12.55 | 50.2 | 21.8 |  |  |  |  |
| 295 K | 13.43 | 54.7 | 28.3 |  |  |  |  |
| 300 K | 15.02 | 54.7 | 28.8 |  |  |  |  |
| 305 K | 18.58 | 59.2 | 36.4 |  |  |  |  |
| 310 K | 21.42 | 59.2 | 36.3 |  |  |  |  |
| 315 K | 21.09 | 59.2 | 36.0 |  |  |  |  |
|  |  | 60.5 | 40.4 |  |  |  |  |
|  |  | 64.5 | 43.7, 44.7 |  |  |  |  |
|  |  | 64.5 | 46.5 |  |  |  |  |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=18.91$ |  |  |  |  |  |  |  |

Empirical temperature dependence equations:
Wauchope \& Getzen (1972): $\mathrm{R} \cdot \ln \mathrm{x}=-\left[\mathrm{H}_{\mathrm{fus}} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{T} / \mathrm{K})$


FIGURE 4.1.1.13.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for biphenyl.

TABLE 4.1.1.13.2
Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

$$
\begin{align*}
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})  \tag{1a}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)  \tag{2}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})  \tag{3}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{~T} / \mathrm{K})  \tag{4}\\
& \log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{~T} / \mathrm{K})^{2} \tag{5}
\end{align*}
$$

$$
\text { (1) } \quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})
$$

$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
1.

| Chipman \& Peltier 1929 |  |  | 1947 | Bright 1951 | Bradley \& Cleasby 1953 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| isoteniscope-manometer |  | summary | terature data | effusion | effusion |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ |
| 162.5 | 7933 | 70.6 | 133.3 | Data presented in graph | 15.050 .416 |
| 172.3 | 10959 | 101.8 | 666.6 | $25 \quad 0.579$ | 20.7 0.7786 |
| 177.7 | 12799 | 117.0 | 1333 | (interpolated) | 24.7 1.2252 |
| 183.5 | 15705 | 134.2 | 2666 | eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | 24.0 1.1825 |
| 191.6 | 19972 | 152.5 | 5333 | A 10.38 | 24.1 |
| 198.75 | 24691 | 165.2 | 7999 | B 3799 | 27.051 .600 |
| 293.8 | 28504 | 180.7 | 13332 | temp range $4.9-34.5^{\circ} \mathrm{C}$ | 29.15 2.053 |
| 211.25 | 34677 | 204.2 | 26664 |  | 32.45 2.973 |
| 220.05 | 43756 | 229.4 | 53329 | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=72.80$ | $35.05 \quad 3.866$ |
| 229.8 | 56329 | 254.0 | 101325 |  | $37.9 \quad 5.160$ |
| 238.2 | 68901 |  |  |  | $40.55 \quad 6.693$ |
| 247.7 | 85580 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 69.5 |  | 23.05 1.027 |
| 253.7 | 98019 |  |  |  | $36.5 \quad 1.533$ |
| 255.2 | 101178 |  |  |  | $31.25 \quad 2.546$ |
|  |  |  |  |  | $35.9 \quad 4.133$ |
| $\mathrm{bp} /{ }^{\circ} \mathrm{C}$ | 266.25 |  |  |  |  |
| $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=44.99$ |  |  |  |  |  |
|  | at bp |  |  |  | A 11.282 |
|  |  |  |  |  | B 4262 |
| eq. 5 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  | temp range $15-41^{\circ} \mathrm{C}$ |
| A | 7.0220 |  |  |  |  |
| B | 1723 |  |  |  |  |
| C | 245700 |  |  |  |  |
| temp ran | $-322^{\circ} \mathrm{C}$ |  |  |  |  |

2. 

| Radchenko \& K. 1974 |  | Nasir et al. 1980 |  | Burkhard et al. 1984 |  | Cunningham 1930 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Knudsen effusion |  | pressure transducer |  | gas saturation-GC |  | in Boublik et al. 1984 |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 24.9 | 1.433 | 123.0 | 2040 | 5.2 | 0.106 | 69.20 | 104 |
| 31.75 | 2.976 | 143.81 | 4773 | 14.9 | 0.361 | 93.3 | 413 |
| 33.7 | 3.734 | 164.69 | 9962 | 24.7 | 1.15 | 148.7 | 4833 |
| 35.5 | 4.538 | 181.28 | 16447 |  |  | 160.0 | 7239 |
| 37.6 | 5.726 | 200.87 | 28599 | eq. 1 | $\mathrm{P} / \mathrm{Pa}$ | 171.1 | 10548 |
| 39.57 | 6.913 | 223.66 | 51518 | A | 14.840 | 182.2 | 15031 |
| 41.52 | 8.26 | 245.65 | 86254 | B | 4402.1 | 193.3 | 21098 |

TABLE 4.1.1.13.2 (Continued)
2.



FIGURE 4.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for biphenyl.

### 4.1.1.14 4-Methylbiphenyl



Common Name: 4-Methylbiphenyl
Synonym: 4-phenyltoluene
Chemical Name: 4-methylbiphenyl
CAS Registry No: 644-08-6
Molecular Formula: $\mathrm{C}_{13} \mathrm{H}_{12}$
Molecular Weight: 168.234
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
49.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
267.5 (2003)

Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$1.015 \quad\left(27^{\circ} \mathrm{C}\right.$, Weast 1982-83; Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$165.7 \quad\left(27^{\circ} \mathrm{C}\right.$, calculated-density)
206.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.575 ( mp at $49.5^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations.):
1.834, 4.05, $7.03\left(4.9,25,40^{\circ} \mathrm{C}\right.$, generator column-HPLC/GC, Doucette \& Andren 1988a)
$\mathrm{S} /(\mathrm{mol} / \mathrm{L})=9.18 \times 10^{-6} \exp \left(0.038 \cdot \mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ (generator column-GC/ECD, temp range $4.9-40^{\circ} \mathrm{C}$, Doucette \& Andren 1988a); or
$\log x=-1436 /(\mathrm{T} / \mathrm{K})-1.541$; temp. range $4.9-40^{\circ} \mathrm{C}$ (generator column-GC/ECD, Doucette \& Andren 1988a)
Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
4.63 (generator column-HPLC/GC, calculated-group contribution, TSA, Doucette \& Andren 1987)
4.63 (recommended, Sangster 1989, 1994)
4.63 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :

Environmental Fate Rate Constants, $k$ or Half-Lives, $\mathrm{t}_{1 / 2}$ :

Half-Lives in the Environment:

### 4.1.1.15 4,4'-Dimethylbiphenyl



Common Name: 4,4'-Dimethylbiphenyl
Synonym: 4,4'-dimethyl-1,1'-biphenyl
Chemical Name: 4,4'-dimethylbiphenyl
CAS Registry No: 613-33-2
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{14}$
Molecular Weight: 182.261
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
125 (Weast 1982-83; Ruelle \& Kesselring 1997; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
295 (Weast 1982-83; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
194.0 (Ruelle \& Kesselring 1997)
229.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.104 (mp at $125^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations.):
$0.0687,0.175,0.441\left(4.9,25,40^{\circ} \mathrm{C}\right.$, generator column-GC, Doucette \& Andren 1988a)
$\mathrm{S} /(\mathrm{mol} / \mathrm{L})=2.90 \times 10^{-7} \exp \left(0.052 \cdot \mathrm{t}^{\circ} \mathrm{C}\right)$ (generator column-GC/ECD, temp range $4-40^{\circ} \mathrm{C}$, Doucette \& Andren 1988a)
$\log x=-1913 /(\mathrm{T} / \mathrm{K})-1.288$; temp. range $4.9-40^{\circ} \mathrm{C}$ (generator column-GC/ECD, Doucette \& Andren 1988a)
Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
0.931 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
5.09 (generator column-GC/ECD, Doucette \& Andren 1987)
5.09 (recommended, Sangster 1989, 1994)
5.09 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 4.1.1.16 DiphenyImethane



Common Name: Diphenylmethane
Synonym: diphenyl methane, 1,1'-methylenebis-benzene
Chemical Name: diphenylmethane
CAS Registry No: 101-81-5
Molecular Formula: $\mathrm{C}_{13} \mathrm{H}_{12}$
Molecular Weight: 168.234
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
25.4 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
265 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.00592,1.00192 \quad\left(20^{\circ} \mathrm{C}, 25^{\circ} \mathrm{C}\right.$. Dreisbach 1955)
$1.001 \quad\left(26^{\circ} \mathrm{C}\right.$ Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$168.1 \quad\left(27^{\circ} \mathrm{C}\right.$, from density, Stephenson \& Malanowski 1987)
$167.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
206.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Evaporation, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ :
Enthalpy of Sublimation, $\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})$ :
$64.02 \quad$ (Bright 1951)
66.845, $45.34 \quad\left(25^{\circ} \mathrm{C}, \mathrm{bp}\right.$, Dreisbach 1955)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 18.28 (Dreisbach 1955) 18.58 (Parks \& Huffman 1931; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
61.92 (Stephenson \& Malanowski 1987)
62.34, 62.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.991\left(\mathrm{mp}\right.$ at $25.4^{\circ} \mathrm{C}$ )

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
14.10 (shake flask/UV, Andrews and Keefer 1949)
16.40 (Deno \& Berkheimer 1960)
3.76 (Lu et al. 1978)
3.00 (shake flask-nephelometry, Hollifield 1979)
16.19 (lit. mean, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated $*$, are compiled at the end of this section):
$133.3^{*} \quad\left(76.0^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $76.0-264.5^{\circ} \mathrm{C}$, Stull 1947)
1.09 (effusion method, interpolated from reported Antoine eq., Bright 1951)
$\log (\mathrm{P} / \mathrm{mmHg})=9.12-3341 /(\mathrm{T} / \mathrm{K})$; temp range $5.1-26.5^{\circ} \mathrm{C}$ (Antoine eq., effusion, Bright 1951)
2.266 (calculated by formula, Dreisbach 1955)
$\log (\mathrm{P} / \mathrm{mmHg})=7.16125-1944.42 /\left(190.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $150-310^{\circ} \mathrm{C}$ (Antoine eq. for liquid state, Dreisbach 1955)
$3904^{*} \quad\left(151.49^{\circ} \mathrm{C}\right.$, static-differential pressure gauge, measured range $151.49-336.32^{\circ} \mathrm{C}$, Wieczorek \& Kobayashi 1980)
0.0452 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.94201-1668.355 /\left(186.212+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $217.5-282.2^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

```
13100* (457.95 K, vapor-liquid equilibrium, measured range 457.95-581.85 K, Klara et al. 1987)
0.052 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.291-1261/(105 + t/ }\mp@subsup{}{}{\circ}\textrm{C})\mathrm{ ; temp range 217-282 }\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ (Antoine eq., Dean 1985, 1992)
0.0885 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log ( }\mp@subsup{\textrm{P}}{\textrm{L}}{}/\textrm{kPa})=5.8765-1707.9/(-101.15 + T/K); temp range 295-383 K (Antoine eq.-I, Stephenson &
    Malanowski 1987)
log ( }\mp@subsup{\textrm{P}}{\textrm{L}}{}/\textrm{kPa})=6.28615-1944.42/(-83.15+T/K); temp range 423-583 K (Antoine eq.-II, Stephenson &
    Malanowski 1987)
log}(\textrm{P}/\textrm{mmHg})=50.8894-5.2749\times103/(T/K) - 14.246\cdotlog (T/K) - 4.2994 × 10-10.(T/K) + 2.4197 \times 10-6.(T/K)2;
    temp range 298-768 K (vapor pressure eq., Yaws 1994)
1.456* (22.25 ' C, transpiration-GC, measured range -0.95 to 22.25 ' C, Verevkin 1999)
```

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
0.931 (calculated-P/C, Mackay et al. 1992)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :

| 4.14 | (Hansch \& Leo 1979) |
| :--- | :--- |
| 4.22 | (HPLC-RT correlation, Burkhard et al. 1985) |
| 4.33 | (HPLC-RT correlation, Eadsforth 1986) |
| 4.14 | (recommended, Sangster 1989,1994) |
| 4.14 | (recommended, Hansch et al. 1995) |

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 4.1.1.16.1
Reported vapor pressures of diphenylmethane at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |


| Stull 1947 |  | Bright 1951 |  | Wieczorek \& Kobayashi 1980 |  | Verevkin 1999 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | effusion method |  | static-differential pressure gauge |  | transpiration-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 76.0 | 133.3 | Data pre | in graph | 151.49 | 3904 | -0.95 | 0.07946 |
| 107.4 | 666.6 |  |  | 151.77 | 3929 | 5.15 | 0.1584 |
| 122.8 | 1333 |  |  | 158.06 | 4942 | 10.15 | 0.3261 |
| 138.8 | 2666 | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | 164.06 | 6182 | 15.05 | 0.6196 |
| 157.8 | 5333 | A | 9.12 | 170.31 | 7799 | 18.65 | 0.9556 |
| 170.2 | 7999 | B | 3341 | 176.25 | 9487 | 22.25 | 1.456 |
| 186.3 | 13332 | temp ra | - $26.5^{\circ} \mathrm{C}$ | 182.32 | 11487 |  |  |
| 210.7 | 26664 |  |  | 189.57 | 14279 | eq. 1a | $\mathrm{P} / \mathrm{Pa}$ |
| 237.5 | 53329 | $\Delta \mathrm{H}_{\text {subl }} /(\mathrm{kJ}$ | $)=64.015$ | 196.01 | 17435 | A | 36.43 |
| 264.5 | 101325 |  |  | 202.69 | 21342 | B | 10639 |

TABLE 4.1.1.16.1 (Continued)

| Stull 1947 |  | Bright 1951 |  | Wieczorek \& Kobayashi 1980 |  | Verevkin 1999 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| summary of literature data |  | effusion method |  | static-differential pressure gauge |  | transpiration-GC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 26.5 | Klara et al. 1987 |  | 209.7 | 26436 | $\begin{array}{r} \Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=88.48 \\ \text { at } 284.3 \mathrm{~K} \end{array}$ |  |
|  |  |  |  | 217.16 | 32381 |  |  |
|  |  |  |  | 225.99 | 41037 | $\begin{array}{r} \Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=87.63 \\ \text { at } 298.15 \mathrm{~K} \end{array}$ |  |
|  |  |  |  | 232.67 | 58832 |  |  |
|  |  | vapor-liquid equilibrium |  | 247.79 | 70500 |  |  |
|  |  | T/K | P/Pa | 255.23 | 83501 | 30.25 | 3.099 |
|  |  | 457.95 | 13100 | 263.79 | 100021 | 35.05 | 4.653 |
|  |  | 488.05 | 31000 | 264.36 | 100938 | 40.05 | 7.019 |
|  |  | 527.25 | 82720 | 272.29 | 119269 | 44.95 | 10.19 |
|  |  | 560.95 | 168900 | 280.24 | 137819 | 55.05 | 21.63 |
|  |  | 581.85 | 250200 | 288.0 | 1377.37 | 60.05 | 30.55 |
|  |  |  |  | 295.97 | 162025 | 65.15 | 47.05 |
|  |  | eq. 3 | $\mathrm{P} / \mathrm{kPa}$ | 303.88 | 186511 | 70.15 | 67.41 |
|  |  | A | 15.1413 | 311.45 | 218741 |  |  |
|  |  | B | 5078.0 | 320.63 | 253090 | eq. 1a P/Pa |  |
|  |  | C | 53.89 | 336.32 | 298026 | A 27.43 |  |
|  |  |  |  |  |  | B 7981.2 |  |
|  |  |  |  | fitted to Chebyshev Polynomial |  | $\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=66.36$ |  |
|  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |



FIGURE 4.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for diphenylmethane.

### 4.1.1.17 Bibenzyl



Common Name: Bibenzyl
Synonym: 1,2-Diphenylethane, dibenzyl, 1,1'-(1,2-ethanediyl) bis-benzene
Chemical Name: 1,2-diphenylethane
CAS Registry No: 103-29-7
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{14}$
Molecular Weight: 182.261
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
$52.5 \quad$ (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
284 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): $0.9780 \quad\left(25^{\circ} \mathrm{C}\right.$ Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$190.2\left(60^{\circ} \mathrm{C}\right.$, calculated-density, Stephenson \& Malanowski 1987)
$186.4 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
229.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
23.43 (Parks \& Huffman 1931)
30.54 (Stephenson \& Malanowski 1987)
22.73 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
94.14 (Stephenson \& Malanowski 1987)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), $\mathrm{F}: 0.537$ ( mp at $52.5^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
4.37 (shake flask-UV, Andrews \& Keefer 1950b)
4.37 (quoted, Pearlman et al. 1984)
1.89; 0.44 (generator column-HPLC/UV; HPLC-RT correlation, Swann et al. 1983)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
133.3* $\quad\left(86.8^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $86.8-284.0^{\circ} \mathrm{C}$, Stull 1947)
0.198 (effusion method, interpolated from reported Antoine eq., Bright 1951)
$\log (\mathrm{P} / \mathrm{mmHg})=9.86-3783 /(\mathrm{T} / \mathrm{K})$; temp range $17.1-44.2^{\circ} \mathrm{C}$ (Antoine eq., effusion, Bright 1951)
17.1* $\quad\left(60^{\circ} \mathrm{C}\right.$, inclined piston, measured range $60-140^{\circ} \mathrm{C}$, Osborn \& Scott 1980)
$\log (\mathrm{P} / \mathrm{atm})=[1-547.288 /(\mathrm{T} / \mathrm{K})] \times 10^{\wedge}\left\{0.914704-6.08831 \times 10^{-4} \cdot(\mathrm{~T} / \mathrm{K})+5.11258 \times 10^{-7} \cdot(\mathrm{~T} / \mathrm{K})^{2}\right\} ;$ temp range 333.15-413.15 K, (Cox eq., Chao et al. 1983)
0.406 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.319-4386 /(\mathrm{T} / \mathrm{K})$, temp range 286-308 K, (Antoine eq-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.93271-2636.21 /(-22.009+\mathrm{T} / \mathrm{K})$; temp range $369-557 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=48.5573-5.2841 \times 10^{3} /(\mathrm{T} / \mathrm{K})-13.41 \cdot \log (\mathrm{~T} / \mathrm{K})-1.0073 \times 10^{-9} \cdot(\mathrm{~T} / \mathrm{K})+2.1338 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 324-780 K (vapor pressure eq., Yaws 1994)
$0.734 ; 0.249$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3522 /(\mathrm{T} / \mathrm{K})+11.67 ; \Delta \mathrm{H}_{\text {vap }}=-67.4 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.79, 4.82 (Hansch \& Leo 1979)
4.76 (quoted, HPLC-k' correlation, Hammers et al. 1982)
3.67 (HPLC-RT correlation, Swann et al. 1983)
4.60 (HPLC-RT correlation, Webster et al. 1985)
4.71 (HPLC-RT correlation, Eadsworth 1986)
$4.70 \pm 0.20$ (recommended, Sangster 1989)
4.79 (recommended, Sangster 1993)
4.79 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 4.1.1.17.1
Reported vapor pressures of bibenzyl at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  | $(1 \mathrm{a})$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | $(4)$ |  |  |

$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

Stull 1947
Bright 1951
Osborn \& Scott 1980

| summary of literature data |  |
| :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 86.8 | 133.3 |
| 119.8 | 666.6 |
| 136.0 | 1333 |
| 153.7 | 2666 |
| 173.7 | 5333 |
| 186.0 | 7999 |
| 202.8 | 13332 |
| 227.8 | 26664 |
| 255.0 | 53329 |
| 284.0 | 101325 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ |  |
|  |  |


| effusion method | inclined piston |  |
| :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| Data presented in graph | 60 | 17.1 |
|  | 65 | 24.1 |
|  | 70 | 34.0 |
| eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | 75 | 47.7 |
| A 9.56 | 80 | 65.9 |
| B 3783 | 85 | 89.7 |
| temp range $17.1-44.2^{\circ} \mathrm{C}$ | 90 | 121.2 |
|  | 95 | 161.9 |
| $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=72.38$ | 100 | 213.6 |
|  | 105 | 280.1 |
|  | 110 | 364.2 |
|  | 115 | 469.8 |
|  | 120 | 602.4 |
|  | 125 | 761.8 |
|  | 130 | 961.1 |
|  | 135 | 1202.7 |
|  | 140 | 1498 |
|  | ta fitt | -constan |

vapor pressure eq.


FIGURE 4.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for bibenzyl.

### 4.1.1.18 trans-Stilbene



Common Name: trans-1,2-Diphenylethene
Synonym: trans-stilbene, trans-diphenylethylene, E-stilbene
Chemical Name: trans-1,2-diphenylethene
CAS Registry No: 103-30-0
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{12}$
Molecular Weight: 180.245
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
124.2 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
307 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
0.9707 (Weast 1982-83; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
185.0 (Ruelle \& Kesselring 1997)
$185.7 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
221.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Sublimation, $\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})$ :
100.7 (Van Ekeren et al. 1983)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
30.125 (Stephenson \& Malanowski 1987)
27.40 (Ruelle \& Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
76.73 (Stephenson \& Malanowski 1987)
68.81, 69.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.106 ( mp at $124.2^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
0.29 (shake flask-UV, Andrews \& Keefer 1950)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$133.3^{*} \quad\left(113.2^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $113.2-306.5^{\circ} \mathrm{C}$, Stull 1947$)$
0.00764* (manometer-spinning rotor friction gauge, torsion mass loss effusion, measured range 297.45-364.5 K, Van Ekeren et al. 1983)
$0.0274 \quad\left(34.65^{\circ} \mathrm{C}\right.$, effusion-quartz crystal microbalance, Offringa et al. 1983)
0.00647 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.25604-5201.358 /(\mathrm{T} / \mathrm{K})$; temp range $298-343 \mathrm{~K}$ (Antoine eq.-I, solid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.97928-2610.05 /(-54.759+\mathrm{T} / \mathrm{K})$; temp range $419-580 \mathrm{~K}$ (Antoine eq.-II, liquid, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=68.6303-6.3776 \times 10^{3} /(\mathrm{T} / \mathrm{K})-21.015 \cdot \log (\mathrm{~T} / \mathrm{K})+5.7813 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+1.8334 \times 10^{-12} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $397-820 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.81 (Hansch \& Leo 1979)

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4.81 (recommended, Sangster 1989)
4.81 (recommended, Hansch et al. 1995)
```

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
7.48 (calculated- $\mathrm{S}_{\text {oct }}$ and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k , or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 4.1.1.18.1
Reported vapor pressures of trans-stilbene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(4)

Stull 1947 Van Ekeren et al. 1983

| Summary of literature data |  | Spinning rotor fraction gauge |  | Torsion mass loss effusion |  | Static method |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 113.2 | 133.3 | 24.3 | 0.00704 | 44.97 | 0.100 | 69.17 | 1.43 |
| 145.8 | 666.6 | 24.3 | 0.00699 | 50.78 | 0.200 | 69.45 | 1.44 |
| 161.0 | 1333 | 24.3 | 0.00715 | 54.27 | 0.300 | 71.25 | 1.83 |
| 179.8 | 2666 | 24.43 | 0.0693 | 56.80 | 0.400 | 71.52 | 1.80 |
| 199.0 | 5333 | 27.24 | 0.0102 | 60.43 | 0.600 | 72.2 | 1.94 |
| 211.5 | 7999 | 27.24 | 0.0104 | 64.14 | 0.900 | 73.70 | 2.25 |
| 227.4 | 13332 | 27.24 | 0.0105 | 65.11 | 1.00 | 74.18 | 2.39 |
| 251.7 | 26664 | 30.65 | 0.0151 | 69.45 | 1.44 | 75.73 | 2.81 |
| 287.3 | 53329 | 30.65 | 0.015 | 71.25 | 1.83 | 75.83 | 2.80 |
| 306.5 | 101325 | 32.03 | 0.0196 | 71.25 | 1.80 | 75.86 | 2.83 |
|  |  | 32.03 | 0.0195 | 72.2 | 1.94 | 77.15 | 3.10 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 124 | 34.96 | 0.0287 | 73.7 | 2.25 | 78.27 | 3.55 |
|  |  | 34.96 | 0.0288 | 74.18 | 2.39 | 8.06 | 4.34 |
|  |  | 34.96 | 0.0289 | 75.73 | 2.81 | 80.39 | 4.39 |
|  |  | $37.33$ | $0.0386$ | $75.86$ | $2.83$ | $81.79$ | $5.07$ |
|  |  | 37.33 | $0.0387$ | $76.88$ | 3.10 | 83.36 | $5.84$ |
|  |  | 40.61 | 0.0584 | 78.27 | 3.55 | 85.04 | 6.86 |
|  |  | 40.61 | 0.0585 | 80.79 | 4.39 | 86.35 | 7.71 |
|  |  | 43.32 | 0.0792 | 81.79 | 5.07 | 86.38 | 7.74 |
|  |  | 25 | 0.00765 | $83.36$ | $5.84$ | 86.51 | $7.90$ |
|  |  |  |  | $85.04$ | $6.86$ | 87.35 | $8.47$ |
|  |  |  |  | 86.35 | 7.71 | 89.74 | 10.57 |
|  |  |  |  | 86.51 | 7.90 | 90.43 | 11.22 |
|  |  |  |  | 87.35 | 8.47 | 91.35 | 12.20 |
|  |  |  |  | $89.74$ | 10.57 |  |  |
|  |  |  |  | 90.43 | 11.22 |  |  |
|  |  |  |  | 91.35 | 12.20 |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\text {fus }}=$ | $\mathrm{kJ} / \mathrm{mol}$ |  |  |
|  |  |  |  |  |  |  |  |



FIGURE 4.1.1.18.1 Logarithm of vapor pressure versus reciprocal temperature for trans-stilbene.

### 4.1.1.19 Acenaphthylene



Common Name: Acenaphthylene
Synonym:
Chemical Name: acenaphthylene
CAS Registry No: 208-96-8
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{8}$
Molecular Weight: 152.192
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
91.8 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
280 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
0.899 (Dean 1985)
$0.8987 \quad\left(17^{\circ} \mathrm{C}\right.$, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
141.2 (Ruelle \& Kesselring 1997)
$167.1 \quad\left(17^{\circ} \mathrm{C}\right.$, calculated-density)
165.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
10.96 (Ruelle \& Kesselring 1997)
$1.4,6.95,10.96 ; 12.36\left(-156.55,88.45,88.85^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
30.3 (Passivirta et al. 1999)
42.4, 37.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.221 (mp at $91.8^{\circ} \mathrm{C}$ )
0.458 (calculated, $\Delta \mathrm{S}_{\text {fus }}=30.3 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
3.93 (misquoted from Mackay \& Shiu 1977)
16.1 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=1.315-573.5 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.893* (gas saturation-HPLC/fluo./UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=12.768-3821.55 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., Sonnefeld et al. 1983)
0.893 (generator column-HPLC, Wasik et al. 1983)
1.105 (interpolated, Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=9.500-3714 /(\mathrm{T} / \mathrm{K})$; temp range $286-318 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
0.90 (selected, Mackay et al. 1992, 1996; quoted, Shiu \& Mackay 1997)
$0.90 ; 1.97$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.11-3201 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.53-2751 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
11.55 (gas stripping-GC, Warner et al. 1987)
11.40 (wetted-wall column-GC, Fendinger \& Glotfelty 1990)
12.7* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-6278.6 /(\mathrm{T} / \mathrm{K})+15.757 ; \Delta \mathrm{H}=52.2 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=8.22-2178 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.07 (calculated as per Leo et al. 1971)
3.94 (Yalkowsky \& Valvani 1979)
3.72 (calculated-fragment const., Mabey et al. 1982)
4.08 (selected, Mills et al. 1982)
4.06 (calculated-molar refraction MR, Yoshida et al. 1983)
3.90 (calculated-MCI $\chi$ as per Rekker \& De Kort 1979, Ruepert et al. 1985)
3.55 (HPLC-RT correlation, Chin et al. 1986)
4.07-4.10; 4.08 (quoted lit. range; lit. mean, Meadors et al. 1995)
4.00; 3.67 (quoted lit.; calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:

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3.0 (microorganisms-water, calculated-K}\mp@subsup{\textrm{K}}{\mathrm{ Ow }}{}\mathrm{ , Mabey et al. 1982)
2.58 (Isnard & Lambert 1988)
```

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:

| $3.83,3.75$ | (soil, RP-HPLC correlation on CIHAC, on PIHAC, Szabo et al. 1990b) |
| :--- | :--- |
| $4.91-5.21 ; 3.60-3.80$ | (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss |
| \& Wilcke 2001) |  |

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis: not environmentally significant (Mabey et al. 1982);
$\mathrm{t}_{1 / 2}=0.7 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=2.2 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=44 \mathrm{~h}$ on fly ash for different atmospheric particulate substrates determined in the rotary photoreactor (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate) (Behymer \& Hites 1985); direct photolysis $t_{1 / 2}=9.08 \mathrm{~h}$ (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).
Photodegradation $\mathrm{k}=3 \times 10^{-5} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}=4 \times 10^{7} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=5 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (calculated, Mabey et al. 1982)
$\mathrm{k}_{\mathrm{O}_{3}} \sim 5.50 \times 10^{-16} \mathrm{~cm}^{3} \cdot$ molecule ${ }^{-1} \cdot \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}=(11.0 \pm 0.1) \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{NO}_{3}}=(54 \pm 0.8) \times$ $10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate methods, Atkinson \& Aschmann1988)
$\mathrm{k}_{\mathrm{OH}}=11.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 296 K (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=12.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ with a atmospheric lifetime of 1.1 h assuming an average ambient 12 -h daytime OH radical concn of $2 \times 10^{6}$ molecule $/ \mathrm{cm}^{3} ; \mathrm{k}_{\mathrm{O}_{3}}=1.60 \times 10^{-16} \mathrm{~cm}^{3} \cdot \mathrm{molecul}^{-1} \cdot \mathrm{~s}^{-1}$ at 296 K with lifetime of 2.5 h assuming ambient $\mathrm{O}_{3}$ concn of $7 \times 10^{11}$ molecule $/ \mathrm{cm}^{3}$ (relative rate method, Reisen \& Arey 2002)
Hydrolysis: not hydrolyzable (Mabey et al. 1982; Howard et al. 1991).
Biodegradation: $>98 \%$ degradation within 7 d , based on domestic sewer for an average of three static-flask
screening test (Tabak et al. 1981);
aerobic $\mathrm{t}_{1 / 2}=1020-1440 \mathrm{~h}$, based on soil column study data (Kincannon \& Lin 1985; quoted, Howard et al. 1991);
anaerobic $t_{1 / 2}=4080-5760 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation: $\mathrm{k}=3 \times 10^{-9} \mathrm{~mL}$ cell ${ }^{-1} \mathrm{~h}^{-1}$, estimated rate constant for bacteria (Mabey et al. 1982)
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.191-1.27 \mathrm{~h}$, based on photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).
Atmospheric lifetime of 1.1 h and 2.5 h due to reaction with OH and $\mathrm{O}_{3}$ at 296 K , respectively (Reisens \& Arey 2002)
Surface water: $t_{1 / 2}=1020-1440 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Kincannon \& Lin 1985; quoted, Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=2040-2880 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $\mathrm{t}_{1 / 2}=1020-1440 \mathrm{~h}$, based on soil column study data (Kincannon \& Lin 1985; quoted, Howard et al. 1991); $t_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988).
Biota: elimination $\mathrm{t}_{1 / 2}=1 \mathrm{~d}$ from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.19.1
Reported vapor pressures and Henry's law constants of acenaphthlyene at various temperatures and the coefficients for the vapor pressure equations

| Vapor pressure |  | Henry's law constant |  |  |
| :---: | :---: | :---: | :---: | :---: |
| Sonnefeld et al. 1983 |  | Bamford et al. 1999 |  |  |
| gas saturation-HPLC |  | gas stripping-GC/MS |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | $\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ |
|  |  |  |  | average |
| 11.20 | 0.206 | 4.1 | 1.98, 2.87 | 2.38 |
| 11.20 | 0.205 | 11.0 | 3.76. 4.86 | 4.27 |
| 11.20 | 0.216 | 18.0 | 6.67, 8.33 | 7.46 |
| 20.56 | 0.590 | 25.0 | 10.9, 14.6 | 12.7 |
| 20.56 | 0.585 | 31.0 | 16.2, 23.7 | 19.6 |
| 20.56 | 0.588 |  |  |  |
| 30.40 | 1.50 | $\ln$ | - B/(T/K) |  |
| 30.40 | 1.54 | A | 15.7566 |  |
| 30.40 | 1.52 | B | 6278.6 |  |
| 39.05 | 3.30 |  |  |  |
| 39.05 | 3.41 | enthalpy, en | ange: |  |
| 39.05 | 3.27 | $\Delta \mathrm{H} /(\mathrm{kJ} \cdot \mathrm{mol}$ | $2 \pm 3.3$ |  |
| 39.05 | 3.34 | $\Delta \mathrm{S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~m}\right.$ |  |  |
| 25.0 | 0.89 |  | at $25^{\circ} \mathrm{C}$ |  |

$\log \mathrm{P} / \mathrm{Pa}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

| A | 12.768 |
| :--- | :--- |
| B | 3821.55 |



FIGURE 4.1.1.19.1 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for acenaphthylene.

### 4.1.1.20 Acenaphthene



Common Name: Acenaphthene
Synonym: 1,8-hydroacenaphthylene, ethylenenaphthalene, periethylenenaphthalene, 1,2-dihydro-acenaphthalene
Chemical Name: 1,8-hydroacenaphthylene
CAS Registry No: 83-32-9
Molecular Formula: $\mathrm{C}_{12} \mathrm{H}_{10}$
Molecular Weight: 154.207
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
93.4 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
279 (Weast 1982-82; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.069 \quad\left(95^{\circ} \mathrm{C}\right.$, Dean 1985)
1.222 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$126.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
173.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Sublimation, $\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})$ :
84.68 (Radchenko \& Kitiagorodskii 1974)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
21.88 (differential calorimetry, Wauchope \& Getzen 1972)
21.46 (calorimetry, Osborn \& Douslin 1975; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
60.25 (Wauchope \& Getzen 1972)
59.83 (Casellato et al. 1973)
56.90 (Ubbelohde 1978)
58.55, 41.09 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.213 ( mp at $93.4^{\circ} \mathrm{C}$ )
0.197 (calculated, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
6.14 (Deno \& Berkheimer 1960)
3.88* (shake flask-UV, measured range $0-74.7^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-5230 /(\mathrm{T} / \mathrm{K})+4.08 \times 10^{-4} \cdot[(\mathrm{~T} / \mathrm{K})-291.15]^{2}-17.1+0.0186 \cdot(\mathrm{~T} / \mathrm{K})$; temp range $22.2-73.4^{\circ} \mathrm{C}$ (shake flask-UV measurements, Wauchope \& Getzen 1972)
3.59 (shake flask-UV, Vesala 1974)
3.47 (shake flask-GC, Eganhouse \& Calder 1976)
3.93 (shake flask-fluorescence, Mackay \& Shiu 1977)
7.37 (shake flask-LSC, Banerjee et al. 1980)
2.42 (shake flask-GC, Rossi \& Thomas 1981)
4.47 (average lit. value, Pearlman et al. 1984)
4.16 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
3.8* (recommended, IUPAC Solubility Data Series, Shaw 1989)
3.88 (shake flask-HPLC, Haines \& Sandler 1995)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=2.505-1127 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid $\mathrm{S}_{\mathrm{L}}$, Passivirta et al. 1999)
$\ln x=0.684974-4541.77 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2560* $\quad\left(147.2^{\circ} \mathrm{C}\right.$, static isoteniscope method, measured range $147.2-287.8^{\circ} \mathrm{C}$, Mortimer \& Murphy 1923) $\log (\mathrm{P} / \mathrm{mmHg})=8.033-2835 /(\mathrm{T} / \mathrm{K})$; temp range $147.2-287.8^{\circ} \mathrm{C}$ (Antoine eq. static isoteniscope method, Mortimer \& Murphy 1923)
666.6* ( $114.8^{\circ} \mathrm{C}$, summary of literature data, temp range $114.8-277.5^{\circ} \mathrm{C}$, Stull 1947)
0.207 (Hoyer \& Peperle 1958)
$\log (\mathrm{P} / \mathrm{mmHg})=11.50-4264 /(\mathrm{T} / \mathrm{K})$; temp range -15 to $30^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958)
4.02 (extrapolated-Antoine eq., Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 13078.5 /(\mathrm{T} / \mathrm{K})]+8.069478$; temp range $114.8-277.5^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
3.07 (extrapolated-Antoine eq., liquid state $\mathrm{P}_{\mathrm{L}}$, Boublik et al. 1973)
8.622* $\quad\left(54.1^{\circ} \mathrm{C}\right.$, effusion method, measured range $54.1-83.45^{\circ} \mathrm{C}$, Radchenko \& Kitiagorodskii 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=12.2930-4422.921 /(\mathrm{T} / \mathrm{K})$; temp range $54.10-83.15^{\circ} \mathrm{C}$ (Antoine eq., Knudsen effusion,
Radchenko \& Kitiagorodskii 1974)
0.373* (manometry-extrapolated, measured range $65-140^{\circ} \mathrm{C}$, Osborn \& Douslin 1975)
0.287* (gas saturation-HPLC/fluo./UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=14.669-4535.39 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., gas saturation, Sonnefeld et al. 1983)
0.287 (gas saturation/generator column-HPLC, Wasik et al. 1983)
3.03, 1.48 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.84571-2527.716 /\left(244.912+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $147.2-287.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Mortimer \& Murphy 1923, Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.38504-2102.491 /\left(203.124+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $95-140^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data of Osborn \& Douslin 1966, Boublik et al. 1984)
3.07 (extrapolated from liquid state $\mathrm{P}_{\mathrm{L}}$, Dean 1985)
$\log (\mathrm{P} / \mathrm{mmHg})=7.72819-2534.234 /\left(245.576+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $147-187^{\circ} \mathrm{C}$ (Antoine eq., Dean 1885,1992 )
$\log (\mathrm{P} / \mathrm{mmHg})=8.033-2834.99 /(\mathrm{T} / \mathrm{K})$; temp range $147-288^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$0.237,0.319 \quad\left(19.95^{\circ} \mathrm{C}, 26.85^{\circ} \mathrm{C}\right.$, gas saturation-GC, Sato al. 1986)
0.427* (gas saturation, interpolated-Antoine eq., temp range $20-169^{\circ} \mathrm{C}$, Sato al. 1986)
$\ln (\mathrm{P} / \mathrm{Pa})=22.9288-5183.86 /(\mathrm{T} / \mathrm{K}-80.153)$; temp range: 293.1-342 K (Antoine eq., gas saturation, Sato et al. 1986)
0.311 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.883-4290.5 /(\mathrm{T} / \mathrm{K})$; temp range $290-311 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=9.4944-3248.008 /(-48.055+\mathrm{T} / \mathrm{K})$; temp range $338-366 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.3519-2082.356 /(-71.578+\mathrm{T} / \mathrm{K})$; temp range $368-413 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.30401-2975 /(10.674+\mathrm{T} / \mathrm{K})$; temp range $388-552 \mathrm{~K}$ (Antoine eq.-IV, Stephenson \& Malanowski 1987)
$0.336,0.211,0.383 ; 0.287 ; 0.375 ; 0.377,0.122,0.306,0.862$ (quoted lit. values: effusion method; gas saturationHPLC; calculated, Delle Site 1997)
$0.30 ; 1.52$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.20-3492 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=8.13-2367 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{kPa})=10.883-4290.5 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000) 1.52; 0.428 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3337 /(\mathrm{T} / \mathrm{K})+11.37 ; \Delta \mathrm{H}_{\mathrm{V} .}=-63.9 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):

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14.79 (gas stripping-GC, Mackay et al. 1979)
15.7 (gas stripping-GC, Mackay & Shiu 1981; Mackay et al. 1982)
24.42 (gas stripping-GC, Warner et al. 1987)
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6.45 (wetted-wall column-GC, Fendinger \& Glotfelty 1990)
9.17 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
16.20 (gas stripping-fluorescence, Shiu \& Mackay 1997)
18.5* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-6242.48 /(\mathrm{T} / \mathrm{K})+16.0, \Delta \mathrm{H}=51.9 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$, (gas stripping-GC, Bamford et al. 1999)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=5.63-1240 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
3.92 (shake flask-LSC, Veith et al. 1979, 1980)
3.92; 4.49 (shake flask-GC; RP-HPLC-RT correlation; Veith et al. 1980)
$3.92 \quad\left(23^{\circ} \mathrm{C}\right.$, shake flask, Banerjee et al. 1980)
3.92 (recommended, Sangster 1989, 1993)
3.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ :
6.31 (calculated- $S_{\text {oct }}$ and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log \mathrm{BCF}$ :
2.59 (bluegill sunfish, Veith et al. 1979, 1980)
2.59 (bluegill sunfish, Barrows et al. 1980)
2.59 (bluegill sunfish, Davies \& Dobbs, 1984)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
5.38 (sediments average, Kayal \& Connell 1990)
3.79 (RP-HPLC correlation on CIHAC, Szabo 1990b)
3.59 (RP-HPLC correlation on PIHAC, Szabo 1990b; quoted, Pussemier et al. 1990)
3.58; 3.79 (HPLC-screening method; calculated-PCKOC fragment method, Müller \& Kördel 1996)
3.40-5.33; 3.80-5.40 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
4.79; $4.89,4.31,4.20 \quad\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: half-lives on different atmospheric substrates determined in the rotary photoreactor (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=2.0 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=2.2 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=44 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985); $\mathrm{k}=0.23 \mathrm{~h}^{-1}$ in distilled water with $\mathrm{t}_{1 / 2}=3 \mathrm{~h}$ (Fukuda et al. 1988);
direct photolysis $t_{1 / 2}=7.67 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).
Hydrolysis: not hydrolyzable (Mabey et al. 1982).
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}<3600 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet $\mathrm{O}_{2}, \mathrm{k}=8000 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical at $25^{\circ} \mathrm{C}$ (Mabey et al. 1982)
$\mathrm{k}_{\mathrm{OH}}($ exptl $)=1.03 \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=1.49 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (Atkinson et al. 1988) $\mathrm{k}_{\mathrm{O}_{3}}<5.0 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$, $\mathrm{k}_{\mathrm{OH}}=(1.03 \pm 0.13) \times 10^{-10} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{NO}_{3}}=$
$(4.6 \pm 2.6) \times 10^{-13} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ (relative rate methods, Atkinson \& Aschmann1988)
$\mathrm{k}_{\mathrm{OH}}=(103-58.4) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296-300 \mathrm{~K}$ (Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=84.03 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}} *=58 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $325-365 \mathrm{~K}$ with a calculated atmospheric lifetime of 4.9 h based on gas-phase OH reaction (Brubaker \& Hites 1998)
$\mathrm{k}_{\mathrm{OH}}=8.9 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $296 \pm 2 \mathrm{~K}$ with a atmospheric lifetime of 1.8 h assuming an average ambient 12-h daytime OH radical concn of $2 \times 10^{6}$ molecule $/ \mathrm{cm}^{3}$ (Reisen \& Arey 2002)
Biodegradation: significant degradation within 7 d for a domestic sewer test (Tabak et al. 1981);
aerobic $t_{1 / 2}=295-2448 \mathrm{~h}$, based on aerobic soil column test data (Kincannon \& Lin 1985; quoted, Howard et al. 1991);
anaerobic $t_{1 / 2}=1180-9792 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation: $3 \times 10^{-9} \mathrm{~mL}^{\text {cell }}{ }^{-1} \mathrm{~h}^{-1}$, estimated bacterial transformation rate constant (Mabey et al. 1982). Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Sorption $\left(\mathrm{k}_{1}\right)$-Desorption $\left(\mathrm{k}_{2}\right)$ Rate constants: desorption rate constant of $0.018 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=38.5 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.879-8.79 \mathrm{~h}$, based on estimated photooxidation half-life in air (Howard et al. 1991); calculated atmospheric lifetime of 4.9 h based on gas-phase OH reactions (Brubaker \& Hites 1998).
Surface water: $\mathrm{t}_{1 / 2}=3-300 \mathrm{~h}$, based on photolysis half-life in water (Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=590-4896 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: desorption $\mathrm{t}_{1 / 2}=38.5 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $\mathrm{t}_{1 / 2}=295-2448 \mathrm{~h}$, based on aerobic soil column test data (Kincannon \& Lin 1985; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988).
Biota: $\mathrm{t}_{1 / 2}<1.0 \mathrm{~d}$ in the tissue of bluegill sunfish (Veith et al. 1980).

TABLE 4.1.1.20.1
Reported aqueous solubilities of acenaphthene at various temperatures

Wauchope \& Getzen 1972

| shake flask-UV |  |  |  | IUPAC recommended |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  | experimental | smoothed data |  |  |  |
| 22.2 | 3.57 | 0 | 1.45 | 0 | 1.5 |
| 30.0 | 4.76 | 22.2 | 3.46 | 20 | 3.2 |
| 30.0 | 4.60 | 25.0 | 3.88 | 25 | 3.8 |
| 30.0 | 4.72 | 30.0 | 4.80 | 30 | 4.8 |
| 34.5 | 6.00 | 34.5 | 5.83 | 40 | 7.4 |
| 34.5 | 5.68 | 39.3 | 7.20 | 50 | 9.2 |
| 34.5 | 5.75 | 44.7 | 9.20 | 60 | 19 |
| 39.3 | 6.80 | 50 | 11.9 | 70 | 32 |
| 39.3 | 7.10 | 50.1 | 11.9 | 75 | 43 |
| 39.3 | 7.00 | 55.6 | 15.6 |  |  |
| 44.7 | 9.40 | 64.5 | 24.3 |  |  |
| 44.7 | 9.40 | 65.2 | 25.2 |  |  |
| 44.7 | 9.30 | 69.8 | 32.1 |  |  |
| 50.1 | 12.5 | 71.9 | 35.9 |  |  |
| 50.1 | 12.4 | 73.4 | 39.0 |  |  |
| 50.1 | 12.4 | 74.7 | 41.8 |  |  |
| 55.6 | 15.8 | 75.0 | 42.5 |  |  |
| 55.6 | 16.3 |  |  |  |  |
| 55.6 | 15.9 |  |  |  |  |
| 64.5 | 25.9 | tem | nce eq. 1 |  |  |
| 64.5 | 27.8 | $\ln x$ | mole fraction |  |  |
| 65.2 | 23.7 | $\Delta \mathrm{H}_{\text {fus }}$ | $21.88 \pm 0.21$ |  |  |
| 65.2 | 23.4 | $10^{2} \cdot \mathrm{~b}$ | $1.86 \pm 0.11$ |  |  |
| 65.2 | 22.8 | c | $20.8 \pm 0.4$ |  |  |
| 69.8 | 30.1 |  |  |  |  |
| 69.8 | 34.3 |  |  |  |  |

TABLE 4.1.1.20.1 (Continued)

| Wauchope \& Getzen 1972 |  |  |  | Shaw 1989 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  |  |  | IUPAC recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\prime}{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 69.8 | 33.6 |  |  |  |  |
| 71.9 | 35.2 |  |  |  |  |
| 73.4 | 39.1 |  |  |  |  |
| 79.4 | 40.1 |  |  |  |  |
| 74.7 | 40.8 |  |  |  |  |
| 74.7 | 39.3 |  |  |  |  |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=21.88$ |  |  |  |  |  |

Empirical temperature dependence equations:
Wauchope \& Getzen (1972): $\mathrm{R} \cdot \ln x=-\left[\mathrm{H}_{\mathrm{fus}} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{T} / \mathrm{K})$


FIGURE 4.1.1.20.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for acenaphthene.

TABLE 4.1.1.20.2
Reported vapor pressures of acenaphthene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
1.

| Mortimer \& Murphy 1923 |  | Stull 1947 |  | Hoyer \& Peperle 1958 | Radchenko \& K. 1974 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| static isoteniscope method |  | summary of literature data |  | effusion | effusion method |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 147.2 | 2560 | 114.8 | 666.6 | data presented as | 54.1 | 8.622 |
| 182.4 | 8479 | 131.2 | 1333 | eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | 57.85 | 10.576 |
| 182.4 | 8479 | 148.7 | 2666 | A 11.50 | 58.95 | 13.180 |
| 210.2 | 19732 | 168.2 | 5333 | B 4264 | 61.3 | 16.545 |
| 210.4 | 19865 | 181.2 | 7999 | temp range $-15-35^{\circ} \mathrm{C}$ | 64.55 | 20.438 |
| 227.2 | 31277 | 197.5 | 13332 | $\Delta \mathrm{H}_{\text {sub }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=83.26$ | 67.25 | 26.757 |
| 233.2 | 36264 | 222.1 | 26664 |  | 69.5 | 31.304 |
| 246.2 | 49943 | 250.0 | 53329 |  | 71.8 | 37.77 |
| 246.6 | 50383 | 277.5 | 101325 |  | 73.65 | 47.22 |
| 247.0 | 51049 |  |  |  | 76.0 | 57.23 |
| 252.4 | 57929 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 55 |  | 78.05 | 67.66 |
| 252.5 | 57955 |  |  |  | 80.5 | 82.045 |
| 264.4 | 76047 |  |  |  | 83.45 | 130.30 |
| 264.4 | 76460 |  |  |  |  |  |
| 275.3 | 97779 |  |  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |
| 275.4 | 97779 |  |  |  | A | 12.2930 |
| 275.4 | 97779 |  |  |  | B | 4222.924 |
| 286.8 | 124030 |  |  |  |  |  |
| 287.0 | 124296 |  |  |  |  |  |
| 287.8 | 125723 |  |  |  |  |  |
| eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  |  |
| A | 8.033 |  |  |  |  |  |
| B | 2835 |  |  |  |  |  |
| temp range $147-288^{\circ} \mathrm{C}$ |  |  |  |  |  |  |

2. 

| Osborn \& Douslin 1975 |  | Sonnefeld et al. 1983 |  | Sato et al. 1986 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| inclined-piston manometry |  | gas saturation-HPLC |  | gas saturation-electrobalance |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| solid |  |  |  |  |  |
| 65.0 | 25.865 | 10.87 | 0.048 | 19.95 | 0.237 |
| 70.0 | 30.797 | 10.87 | 0.0504 | 26.85 | 0.519 |
| 75.0 | 46.796 | 10.87 | 0.0515 | 30.85 | 0.792 |
| 80.0 | 70.526 | 20.45 | 0.167 | 35.75 | 1.30 |
| 85.0 | 104.92 | 20.45 | 0.161 | 37.95 | 1.60 |
| 90.0 | 153.45 | 20.45 | 10.66 | 43.35 | 3.21 |
| 92.0 | 185.05 | 30.15 | 0.539 | 45.35 | 4.21 |
| 92.5 | 195.05 | 30.15 | 0.512 | 48.35 | 5.76 |

## TABLE 4.1.1.20.2 (Continued)

| Osborn \& Douslin 1975 |  | Sonnefeld et al. 1983 |  | Sato et al. 1986 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| inclined-piston manometry |  | gas saturation-HPLC |  | gas saturation-electrobalance |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| liquid |  | 32.15 | 0.580 | 51.85 | 7.68 |
| 95.0 | 214.91 | 38.9 | 1.35 | 58.05 | 9.72 |
| 100.0 | 281.04 | 38.9 | 1.32 | 60.25 | 12.0 |
| 105.0 | 364.23 | 38.9 | 1.32 | 63.65 | 15.6 |
| 110.0 | 468.35 | 25 | 0.287 | 68.85 | 23.5 |
| 115.0 | 597.94 |  |  |  |  |
| 120.0 | 755.39 | eq. 1 | $\mathrm{P} / \mathrm{Pa}$ | eq. 3 | $\mathrm{P} / \mathrm{Pa}$ |
| 125.0 | 948.97 | A | 14.385 | A | 22.9288 |
| 130.0 | 1184 | B | 4616.07 | B | 5183.86 |
| 135.0 | 1469 |  |  | C | -80.153 |
| 140.0 | 1809 |  |  |  |  |



FIGURE 4.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for acenaphthene.

## TABLE 4.1.1.20.3

Reported Henry's law constants of acenaphthene at various temperatures

|  | Bamford et al. |  |
| :---: | :---: | :---: |
| gas stripping-GC/MS |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
|  |  | average |
| 4.1 | 3.27, 3.79 | 3.52 |
| 11.0 | 5.98, 6.62 | 6.29 |
| 18.0 | 10.5, 11.4 | 10.9 |
| 25.0 | 17.5, 19.6 | 18.5 |
| 31.0 | 26.5, 30.8 | 28.6 |
| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  |
|  | $\mathrm{K}_{\text {AW }}$ |  |
| A | 15.997 |  |
| B | 6242.5 |  |
| enthalpy, entropy change: |  |  |
| $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=51.9 \pm 1.3$ |  |  |
| $\Delta \mathrm{S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=133$ |  |  |



FIGURE 4.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for acenaphthene.

### 4.1.1.21 Fluorene



Common Name: Fluorene
Synonym: 2,3-benzindene, diphenylenemethane, 9H-fluorene
Chemical Name: diphenylenemethane
CAS Registry No: 86-73-7
Molecular Formula: $\mathrm{C}_{13} \mathrm{H}_{10}$
Molecular Weight: 166.218
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
114.77 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
295 (Dean 1985; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.203 \quad\left(0^{\circ} \mathrm{C}\right.$, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
138.0 (calculated-density, liquid molar volume, Lande \& Banerjee 1981)
187.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
19.54 (Wauchope \& Getzen 1972)
19.58 (Osborn \& Douslin 1975; Ruelle \& Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
50.63 (Wauchope \& Getzen 1972)
48.53 (Casellato et al. 1973)
50.48, 51.0 (exptl., calculated-group additivity method, Chickos et al. 1999)
50.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.132 (mp at $114.77^{\circ} \mathrm{C}$ ) 0.161 (calculated, $\Delta \mathrm{S}_{\text {fus }}=50.5 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
1.90 (Pierotti et al. 1959)
1.66 (shake flask, binding to bovine serum albumin, Sahyun 1966)
1.90* (shake flask-UV, measured range $24.6-73.4^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-4670 /(\mathrm{T} / \mathrm{K})+4.08 \times 10^{-4} \cdot[(\mathrm{~T} / \mathrm{K})-291.15]^{2}-24.2+0.0309 \cdot(\mathrm{~T} / \mathrm{K})$; temp range $24.6-73.4^{\circ} \mathrm{C}$ (shake flask-UV measurements, Wauchope \& Getzen 1972)
1.98 (shake flask-fluorescence, Mackay \& Shiu 1977)
1.68* (generator column-HPLC, measured range $6.6-31^{\circ} \mathrm{C}$, May et al. 1978)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=324.0+5.413 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+0.8059 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0025 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $4-29^{\circ} \mathrm{C}$ (generator columnHPLC/UV, May et al. 1978)
$1.62^{*} \quad\left(24^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range 279.75-304.25 K, May et al. 1983)
1.68 (generator column-HPLC, Wasik et al. 1983)
1.83 (average lit. value, Pearlman et al. 1984)
1.90 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
1.96 (generator column-HPLC/UV, Billington et al. 1988)
1.9* (recommended, IUPAC Solubility Data Series, Shaw 1989)
2.23 (generator column-HPLC, Vadas et al. 1991)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=1.664-1024 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=0.82861-4824 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$2400^{*} \quad\left(161.0^{\circ} \mathrm{C}\right.$, static isoteniscope method, measured range $161.0-300.4^{\circ} \mathrm{C}$, Mortimer \& Murphy 1923) $\log (\mathrm{P} / \mathrm{mmHg})=8.059-2957 /(\mathrm{T} / \mathrm{K})$; temp range $161-300.4^{\circ} \mathrm{C}$ (Antoine eq., static isoteniscope method, Mortimer \& Murphy 1923)
$666.6^{*} \quad\left(129.3^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $129.3-295.0^{\circ} \mathrm{C}$, Stull 1947)
$0.087^{*} \quad$ (effusion method, measured range $33.3-49.55^{\circ} \mathrm{C}$, Bradley \& Cleasby 1953)
$\log (\mathrm{P} / \mathrm{cmHg})=10.325-4324 /(\mathrm{T} / \mathrm{K})$; temp range $33.3-49.55^{\circ} \mathrm{C}$ (Antoine eq., Bradley \& Cleasby 1953)
1.66 (extrapolated-Antoine eq., liquid state $\mathrm{P}_{\mathrm{L}}$, Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 13682.8 /(\mathrm{T} / \mathrm{K})]+8.18894$; temp range $129.3-295^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
1.13 (extrapolated-Antoine eq., liquid state $\mathrm{P}_{\mathrm{L}}$, Boublik et al. 1973)
1.133 (extrapolated-Antoine eq., supercooled liquid $P_{L}$, Dean 1985)
0.127* (static method-manometry, measured range $75.8-114^{\circ} \mathrm{C}$, Osborn \& Douslin 1975)
0.0946 (Irwin 1982)
0.080* (gas saturation-HPLC/UV, measured range $10-50^{\circ} \mathrm{C}$, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=14.385-4616.07 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., Sonnefeld et al. 1983)
0.080 (generator column-HPLC, Wasik et al. 1983)
$0.473,0.380 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
$\log (\mathrm{P} / \mathrm{kPa})=2.88490-2635.371 /\left(243.022+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $161-300.4^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
0.403 (Yamasaki et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.7619-2637.1 /\left(243.2+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $161-300^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
$0.0875^{*} \quad$ (gas saturation, interpolated-Antoine eq. derived from exptl. data, temp range $34-72^{\circ} \mathrm{C}$, Sato et al. 1986)
$\ln (\mathrm{P} / \mathrm{Pa})=17.0935-2815.52 /(\mathrm{T} / \mathrm{K}-153.984)$; temp range $307.7-347.5 \mathrm{~K}$ (Antoine eq., gas saturation, Sato et al. 1986)
0.088 (extrapolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.449-4324 /(\mathrm{T} / \mathrm{K})$; temp range $306-323 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.04542-4122.908 /(\mathrm{T} / \mathrm{K})$; temp range $348-388 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.31368-4133.08 /(86.582+\mathrm{T} / \mathrm{K})$; temp range $402-568 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987)
$0.0850^{*}, 0.566$ (pressure gauge in vacuum cell: solid $\mathrm{P}_{\mathrm{S}}$, supercooled liquid $\mathrm{P}_{\mathrm{L}}$, extrapolated for $25^{\circ} \mathrm{C}$ from reported Antoine eq., measured temp range $30.03-154.81^{\circ} \mathrm{C}$, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=11.64431-4268.644 /\left(262.656+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $30.03-100.08^{\circ} \mathrm{C}$ (Antoine eq., pressure gauge, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=7.74839-2641.73 /\left(230.963+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $110.06-154.83^{\circ} \mathrm{C}$ (Antoine eq., pressure gauge, Sasse et al. 1988)
$0.474 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)
0.793 , 0.652 (supercooled $\mathrm{P}_{\mathrm{L}}$ converted from literature Ps with different $\Delta \mathrm{S}_{\text {fus }}$ values, Hinckley et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=53.9382-5.322 \times 10^{3} /(\mathrm{T} / \mathrm{K})-16.059 \cdot \log (\mathrm{~T} / \mathrm{K})+4.5696 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})+8.1430 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2}$; temp range $388-870 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
0.407 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$0.0575,0.0885 ; 0.080 ; 0.0851$ (quoted exptl.: effusion method; gas saturation; manometry, Delle Site 1997) $0.0792,0.243 ; 0.00594,0.00477$ (quoted lit.; calculated; GC-RT correlation, Delle Site 1997)
0.72; 0.116 (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.27-3638 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=8.63-2614 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{Pa})=14.385-4616.07 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000) 0.526; 0.194 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3492 /(\mathrm{T} / \mathrm{K})+11.43 ; \Delta \mathrm{H}_{\text {vap }} .=-66.9 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
$0.086^{*} \quad\left(25.05^{\circ} \mathrm{C}\right.$, transpiration method, measured range $288.7-359.2 \mathrm{~K}$, Verevkin 2004)
$\ln (\mathrm{P} / \mathrm{Pa})=298.47 / \mathrm{R}-95086.65 /[\mathrm{R}(\mathrm{T} / \mathrm{K})]-(30.2 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]$; temp range $288.7-359.2 \mathrm{~K}$ (transpiration method, Verevkin 2004)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
7.75 (batch stripping, Mackay \& Shiu 1981)
10.13 (batch stripping, Mackay et al. 1982)
11.85 (batch stripping, Warner et al. 1987)
6.45 (wetted-wall column, Fendinger \& Glotfelty 1990)
9.75 (gas stripping-fluorescence, Shiu \& Mackay 1997)
6.50 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)
9.81* (gas stripping-GC; measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-5869.62 /(\mathrm{T} / \mathrm{K})+14.193 ; \Delta \mathrm{H}=48.8 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left(\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right)=6.97-1590 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.18 (Hansch \& Leo 1979)
4.12 (Chou \& Jurs 1979)
4.18 (HPLC-k' correlation, Rekker \& De Kort 1979)
3.91 (HPLC- $k^{\prime}$ correlation, Hanai et al. 1981)
4.18 (RP-TLC-k' correlation, Bruggeman et al. 1982)
4.18 (shake flask-UV, Yalkowsky et al. 1983b)
4.23 (HPLC-RT correlation, Rapaport et al. 1984)
4.18 (shake flask-GC, Haky \& Leja 1986)
4.10 (RP-HPLC-RT correlation, Chin et al. 1986)
4.23 (HPLC-RT correlation, Wang et al. 1986)
4.13 (TLC-RT correlation, De Voogt et al. 1990)
4.18 (recommended, Sangster 1993)
4.18 (recommended, Hansch et al. 1995)
$4.32 \pm 0.19,3.68 \pm 0.62 \quad$ (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equation.
Additional data at other temperatures designated $*$ are compiled at the end of this section:
6.68 (calculated, Finizio et al. 1997)
$6.79 *$; 6.59 (generator column-GC; calculated- $\mathrm{C}_{\mathrm{O}} / \mathrm{C}_{\mathrm{A}}$, measured range $0-40^{\circ} \mathrm{C}$, Harner \& Bidleman 1998) $\log \mathrm{K}_{\mathrm{OA}}=-7.74+4332 /(\mathrm{T} / \mathrm{K})$; temp range $0-40^{\circ} \mathrm{C}$ (generator column-GC. Harner \& Bidleman 1998)
6.83, 6.79 (calculated $-S_{\text {oct }}$ and vapor pressure $P$, quoted lit., Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
3.67 (microorganisms-water, calculated- $\mathrm{K}_{\mathrm{Ow}}$, Mabey et al. 1982)
2.70 (Daphnia magna, Newsted \& Giesy 1987)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
3.95; 3.87 (Aldrich and Fluka humic acids, observed; predicted, Chin et al. 1989)
5.47 (sediments average, Kayal \& Connell 1990)
3.76 (RP-HPLC correlation, Pussemier et al. 1990)
4.15, 4.21 (RP-HPLC correlation on CIHAC, on PIHAC, Szabo 1990b)
4.68 (humic acid, HPLC-k' correlation, Nielsen et al. 1997)
3.24-5.75; 4.10-5.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
4.81; 4.93, 4.24, 4.63 $\quad\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss \& Wilcke 2001)
3.95 (Askov soil, a Danish Agricultural soil, Sverdrup et al. 2002)
3.93-6.19 (sediment/water, initial-final values of 5-100 d contact time, gas-purge technique-HPLC/fluo., ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :

Volatilization:
Photolysis: half-lives on different atmospheric particulate substrates determined in rotary photoreactor (approx. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=110 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=62 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=37 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985);
photolysis rate $\mathrm{k}<2 \times 10^{-5} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}>1.6 \mathrm{~d}$ (Kwok et al. 1997):
direct photolysis $t_{1 / 2}=7.69 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)
Photodegradation $\mathrm{k}=9.0 \times 10^{-7} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002).
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}}^{3}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated *data at other temperatures and/or the Arrhenius expression see reference:
k (calc) $<360 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=3 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=13.0 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 300 K (SAR structure-activity relationship, Arey et al. 1989, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=9.90 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculation, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}}(\operatorname{exptl})=(16 \pm 5) \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}, \mathrm{k}_{\mathrm{OH}}(\mathrm{calc})=9.2 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated lifetime $\tau=9 \mathrm{~h} ; \mathrm{k}_{\mathrm{NO}_{3}}($ exptl $)=(3.5 \pm 1.2) \times 10^{-14} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated lifetime $\tau=1.3 \mathrm{~d}$; and $\mathrm{k}_{\mathrm{O}_{3}}($ exptl $)<2 \times 10^{-19} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ with a calculated lifetime $\tau>82 \mathrm{~d}$ at $297 \pm 2 \mathrm{~K}$ (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=23 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $306-366 \mathrm{~K}$ with a calculated atmospheric lifetime of 22 h based on gas-phase OH reactions (Brubaker \& Hites 1998)
Hydrolysis: no hydrolyzable groups (Howard et al. 1991).
Biodegradation: significant degradation with gradual adaptation within 7 d for an average of three static-flask screening test (Tabak et al. 1981);
nonautoclaved groundwater samples of approx. $0.06 \mathrm{mg} / \mathrm{L}$ are degraded at rates of about $30 \%$ per week by microbes (Lee et al. 1984);
$\mathrm{t}_{1 / 2}$ (aq. aerobic) $=768-1440 \mathrm{~h}$, based on aerobic soil die-away test data (Coover \& Sims 1987; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=3072-5760 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation halflife (Howard et al. 1991).
Biotransformation: estimated rate constant for bacteria, $3 \times 10^{-9} \mathrm{~mL}^{\mathrm{cell}}{ }^{-1} \mathrm{~h}^{-1}$ (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=12.3 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.051 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $t_{1 / 2}=6.81-68.1 \mathrm{~h}$, based on reported rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);
photolysis $\mathrm{t}_{1 / 2}>1.6 \mathrm{~d}$; calculated tropospheric lifetimes of $9 \mathrm{~h}, 1.3 \mathrm{~d}$ and $>82 \mathrm{~d}$ due to reactions with OH radical, $\mathrm{NO}_{3}$ radical and $\mathrm{O}_{3}$, respectively, at room temp. (Kwok et al. 1997);
calculated atmospheric lifetime of 22 h based on gas-phase reactions with OH radical (Brubaker \& Hites 1998).

Surface water: $t_{1 / 2}=768-1440 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=1536-2880 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $\mathrm{t}_{1 / 2}=768-1440 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991); $\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988).
Biota: elimination $t_{1 / 2}=7 \mathrm{~d}$ from rainbow trout (quoted, Meador et al. 1995).

TABLE 4.1.1.21.1
Reported aqueous solubilities of fluorene at various temperatures

| Wauchope \& Getzen 1972 |  |  |  | May 1980, 1983 |  | Shaw 1989 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  |  |  | generator column-HPLC |  | IUPAC recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | S/g.m $\mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  | experimental |  | smoothed |  |  |  |  |
| 24.6 | 1.93 | 0 | 0.66 | 6.60 | 0.7184 | 0 | 0.70 |
| 24.6 | 1.87 | 24.6 | 1.86 | 13.2 | 0.9673 | 25 | 1.90 |
| 24.6 | 1.88 | 25 | 1.90 | 18.0 | 1.203 | 30 | 2.40 |
| 29.9 | 2.41 | 29.9 | 2.37 | 24.0 | 1.616 | 40 | 3.80 |
| 29.9 | 2.33 | 30.3 | 2.41 | 27.0 | 1.845 | 50 | 6.30 |
| 29.9 | 2.34 | 38.4 | 3.53 | 31.1 | 2.248 | 60 | 10 |
| 30.3 | 2.10 | 40.1 | 3.84 |  |  | 70 | 19 |
| 30.3 | 2.25 | 47.5 | 5.54 |  |  |  |  |
| 30.3 | 2.23 | 50 | 6.29 | temp d | ce eq. 2 |  |  |
| 38.4 | 3.72 | 50.1 | 6.32 | S | $\mu \mathrm{g} / \mathrm{kg}$ |  |  |
| 38.4 | 3.73 | 50.2 | 6.35 | a | 0.0185 |  |  |
| 40.1 | 3.88 | 54.7 | 8.02 | b | 0.4543 |  |  |
| 40.1 | 3.84, 3.85 | 59.2 | 10.2 | c | 22.76 |  |  |
| 47.5 | 5.59, 5.62 | 60.5 | 10.9 | d | 543.3 |  |  |
| 47.5 | 5.68 | 65.1 | 14.1 |  |  |  |  |
| 50.1 | 6.31, 6.42 | 70.7 | 19.2 | $\Delta \mathrm{H}_{\text {sol }} /$ (k | $=32.97$ |  |  |
| 50.1 | 6.54 | 71.9 | 20.6 | measured | n $5-30^{\circ} \mathrm{C}$ |  |  |
| 50.2 | 6.27 | 73.4 | 22.5 |  |  |  |  |
| 54.7 | 8.31, 8.41 | 75 | 24.7 |  |  |  |  |
| 54.7 | 8.56 |  |  |  |  |  |  |
| 59.2 | 10.5 | temp dependence eq. 1 |  |  |  |  |  |
| 60.5 | 10.7 |  |  |  |  |  |  |
| 60.5 | 11.0 | $\ln x$ | mole fraction |  |  |  |  |
| 60.5 | 11.6 | $\Delta \mathrm{H}_{\text {fus }}$ | $19.54 \pm 0.13$ |  |  |  |  |
| 65.1 | 14.2 | $10^{2} \cdot \mathrm{~b}$ | $3.09 \pm 0.1$ |  |  |  |  |
| 65.1 | 14.1 | c | $24.2 \pm 0.3$ |  |  |  |  |
| 70.7 | 18.5 |  |  |  |  |  |  |
| 70.7 | 18.9 |  |  |  |  |  |  |
| 71.9 | 18.8 |  |  |  |  |  |  |
| 73.4 | 21.5 |  |  |  |  |  |  |

$\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=19.54$
Empirical temperature dependence equations:
Wauchope \& Getzen (1972): R•ln $x=-\left[\mathrm{H}_{\text {fus }} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{T} / \mathrm{K})$
May et al. (1978):-S/( $\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}_{1 / 2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}$


FIGURE 4.1.1.21.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for fluorene.

TABLE 4.1.1.21.2
Reported vapor pressures of fluorene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2)
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log P=A-B /(C+T / K)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A} / \mathrm{R}-\mathrm{B} /[\mathrm{R}(\mathrm{T} / \mathrm{K})]-(\mathrm{C} / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15] ; \mathrm{R}-$ gas constant
(1a)
1.

| Mortimer \& Murphy 1923 |  |  | 1947 | Bradley \& Cleasby 1953 |  | Osborn \& Douslin 1975 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| isoteniscope- Hg manometer |  | summary of literature data |  | effusion |  | manometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 161.0 | 2400 | 129.3 | 666.6 | 33.3 | 0.2186 | 75.0 | 15.065 |
| 202.5 | 9266 | 146.0 | 1333 | 37.2 | 0.3333 | 80.0 | 22.264 |
| 203.0 | 9399 | 164.2 | 2666 | 40.3 | 0.4573 | 85.0 | 32.263 |
| 240.0 | 27398 | 185.2 | 5333 | 45.0 | 0.7239 | 90.0 | 47.462 |
| 241.4 | 27784 | 197.8 | 7999 | 49.25 | 1.0906 | 95.0 | 68.26 |
| 276.6 | 64995 | 214.7 | 13332 | 34.85 | 0.2600 | 100.0 | 99.19 |
| 277.1 | 65421 | 240.3 | 26664 | 38.45 | 0.3746 | 105.0 | 141.45 |
| 295.6 | 98499 | 268.6 | 53329 | 42.45 | 0.5546 | 110.0 | 199.98 |
| 295.7 | 98499 | 295.0 | 101325 | 47.75 | 0.9439 | 114.0 | 259.04 |
| 295.7 | 98499 |  |  | 49.55 | 1.1106 |  |  |
| 299.8 | 107231 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 113 |  |  |  |  |
| 300.4 | 108298 |  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | triple point | 387.943 K |
|  |  |  |  | A | $10.325$ |  |  |
|  |  |  |  | B | $4324$ | $\Delta \mathrm{H}_{\text {subl }} /(\mathrm{kJ} \mathrm{m}$ | $\left.{ }^{-1}\right)=81.76$ |
| eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | temp ra | $33-50^{\circ} \mathrm{C}$ |  | at bp |


| Mortimer \& Murphy 1923 |  | Stull 1947 |  | Bradley \& Cleasby 1953 |  | Osborn \& Douslin 1975 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| isoteniscope- Hg manometer |  | summary of literature data |  | effusion |  | manometry |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| A | $\begin{aligned} & \hline 8.059 \\ & 2957 \end{aligned}$ |  |  |  |  | $\Delta \mathrm{H}_{\text {fus }} /(\mathrm{kJ}$ | $=19.58$ |
| temp range $161-300^{\circ} \mathrm{C}$ |  |  |  |  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ}$ | $\begin{array}{r} 62.17 \\ \text { at bp } \end{array}$ |

2. 

| Sonnefeld et al. 1983 |  | Sato et al. 1986 |  | Sasse et al. 1988 |  | Verevkin 2004 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation-HPLC |  | gas saturation-electrobalance |  | electronic manometry |  | transpiration |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | T/K | $\mathbf{P} / \mathbf{P a}$ |
|  |  |  |  | solid |  |  |  |
| 10.5 | 0.0132 | 34.55 | 0.297 | 30.03 | 0.157 | 288.8 | 0.028 |
| 10.5 | 0.0133 | 36.35 | 0.360 | 39.92 | 0.184 | 290.4 | 0.034 |
| 10.5 | 0.013 | 41.15 | 0.620 | 49.88 | 1.241 | 292.4 | 0.044 |
| 20.4 | 0.0425 | 47.45 | 1.21 | 59.92 | 3.426 | 289.6 | 0.031 |
| 20.4 | 0.0438 | 49.85 | 1.53 | 60.03 | 3.533 | 296.2 | 0.067 |
| 20.4 | 0.0451 | 52.35 | 1.95 | 69.93 | 8.746 | 298.2 | 0.086 |
| 30.0 | 0.147 | 55.45 | 2.60 | 79.96 | 20.67 | 300.2 | 0.112 |
| 29.97 | 0.153 | 57.35 | 3.07 | 79.98 | 20.80 | 302.2 | 0.132 |
| 29.97 | 0.146 | 58.75 | 3.88 | 89.99 | 46.26 | 304.3 | 0.166 |
| 38.85 | 0.387 | 63.25 | 4.78 | 89.99 | 46.40 | 306.3 | 0.218 |
| 38.85 | 0.384 | 64.55 | 5.88 | 100.04 | 97.86 | 308.3 | 0.268 |
| 38.85 | 0.382 | 67.25 | 7.38 | 100.08 | 98.93 | 310.2 | 0.328 |
| 38.9 | 0.387 | 69.75 | 9.13 |  |  | 313.3 | 0.449 |
| 38.9 | 0.393 | 71.25 | 10.2 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 314.3 | 0.507 |
| 25.0 | 0.080 | 74.35 | 13.0 | A | 11.64431 | 315.3 | 0.545 |
|  |  |  |  | B | 4268.664 | 317.3 | 0.666 |
| eq. 1 | $\mathrm{P} / \mathrm{Pa}$ | eq. 3 | $\mathrm{P} / \mathrm{Pa}$ | C | 262.656 | 320.3 | 0.930 |
| A | 14.385 | A | 17.0935 | temp range: $30-100.08^{\circ} \mathrm{C}$ |  | 323.4 | 1.245 |
| B | 4616.07 | B | 2815.52 |  |  | 326.5 | 1.645 |
|  |  | C | -153.984 | liquid |  | 329.3 | 2.223 |
|  |  |  |  | 110.06 | 212.5 | 332.3 | 3.103 |
|  |  |  |  | 120.04 | 352.0 | 335.3 | 3.867 |
|  |  |  |  | 120.04 | 353.0 | 338.2 | 4.838 |
|  |  |  |  | 129.97 | 568.6 | 341.2 | 6.552 |
|  |  |  |  | 139.95 | 894.3 | 344.2 | 8.417 |
|  |  |  |  | 149.86 | 1369 | 347.1 | 11.190 |
|  |  |  |  | 154.81 | 1683 | 350.3 | 14.497 |
|  |  |  |  |  |  | 353.2 | 18.302 |
|  |  |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ | 356.3 | 23.900 |
|  |  |  |  | A | 7.94839 | 359.2 | 30.456 |
|  |  |  |  | B | 2641.73 |  |  |
|  |  |  |  | C | 230.963 | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=86.08$ |  |
|  |  |  |  | temp ran |  | eq. 5 | $\mathrm{P} / \mathrm{Pa}$ |
|  |  |  |  |  |  | A | 298.47 |
|  |  |  |  |  |  | B | 95086.65 |
|  |  |  |  |  |  | C | 30.2 |



FIGURE 4.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for fluorene.

TABLE 4.1.1.21.3
Reported Henry's law constants and octanol-air partition coefficients of fluorene at various temperatures and temperature dependence equations

| Henry's law constant |  |  | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {OA }}$ |  |
| :---: | :---: | :---: | :---: | :---: |
| Bamford et al. 1999 |  |  | Harner \& Bidleman 1998 |  |
| gas stripping-GC/MS |  |  | generator column-GC/FID |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | $\boldsymbol{l o g} \mathrm{K}_{\mathrm{OA}}$ |
|  |  | average |  |  |
| 4.1 | 1.96, 2.14 | 2.05 | 0 | 8.134 |
| 11.0 | 3.44, 3.65 | 3.54 | 10 | 7.501 |
| 18.0 | 5.81, 6.12 | 5.96 | 20 | 7.130 |
| 25.0 | 9.49, 10.1 | 9.81 | 30 | 6.516 |
| 31.0 | 14.1, 15.4 | 14.8 | 40 | 6.093 |
|  |  |  | 25(exptl) | 6.79 |
| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | 25(calc) | 6.59 |
| eq. 1 | $\mathrm{K}_{\text {AW }}$ |  |  |  |
| A | 14.193 |  | $\log \mathrm{K}_{\mathrm{OA}}=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| B | 5870 |  | A | -7.74 |
|  |  |  | B | 4332 |
| enthalpy, entropy change: |  |  |  |  |
| $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=48.8 \pm 0.8$ |  |  | enthalpy of phase change |  |
| $\Delta \mathrm{S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=118$ |  |  | $\Delta \mathrm{H}_{\mathrm{OA}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=82.9$ |  |
| at $25^{\circ} \mathrm{C}$ |  |  |  |  |  |



FIGURE 4.1.1.21.3 Logarithm of Henry's law constant and $\mathrm{K}_{\mathrm{OA}}$ versus reciprocal temperature for fluorene.

### 4.1.1.22 1-Methylfluorene



Common Name: 1-Methylfluorene
Synonym:
Chemical Name: 1-methylfluorene
CAS Registry No: 1730-37-6
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{12}$
Molecular Weight: 180.245
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
87 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
318 (Weast 1982)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
177.1 (Ruelle \& Kesselring 1997)
210.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.246\left(\mathrm{mp}\right.$ at $87^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
1.092, 4.867 (measured, supercooled liquid value, Miller et al. 1985)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations):
0.136; 0.0708 (supercooled liquid $P_{L}$ : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3711 /(\mathrm{T} / \mathrm{K})+11.58 ; \Delta \mathrm{H}_{\text {vap }}=-71.1 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
$0.032 \quad\left(24.95^{\circ} \mathrm{C}\right.$, transpiration method, measured range $298.1-375.3 \mathrm{~K}$, Verevkin 2004)
$\ln \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=311.78 / \mathrm{R}-101590.4 /[\mathrm{R}(\mathrm{T} / \mathrm{K})]-(35.1 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]$; temp range 298.1-359.2 K (solid, transpiration method, Verevkin 2004)
$\ln \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=330.39 / \mathrm{R}-104778.1 /[\mathrm{R}(\mathrm{T} / \mathrm{K})]-(87.5 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]$; temp range $361.2-375.3 \mathrm{~K}$ (liquid, transpiration method, Verevkin 2004)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
4.97 (calculated, Miller et al. 1985)
4.63 (calculated-solvatochromic parameters and $\mathrm{V}_{\mathrm{I}}$, Kamlet et al. 1988)
5.7640 (calculated-UNIFAC group contribution, Chen et al. 1993)
4.97 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 4.1.1.23 Phenanthrene



Common Name: Phenanthrene
Synonym: o-diphenyleneethylene, phenanthren
Chemical Name: phenanthrene
CAS Registry No: 85-01-8
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{10}$
Molecular Weight: 178.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
99.24 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
340 (Dean 1985; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
1.174 (Dean 1985)
$0.980 \quad\left(4^{\circ} \mathrm{C}\right.$, Weast 1982-83; Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
182.0 (calculated-density, liquid molar volume, Lande \& Banerjee 1981)
199.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
18.62 (Parks \& Huffman 1931; Tsonopoulos \& Prausnitz 1971; Fu \& Luthy 1985)
16.28 (differential calorimetry, Wauchope \& Getzen 1972)
16.44 (calorimetry, Osborn \& Douslin 1975)
$0.22,16.46 ; 15.58 \quad\left(74.35,99.25^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
42.68 (Wauchope \& Getzen 1972)
45.19 (Casellato et al. 1973)
50.63 (Ubbelohde 1978)
47.70 (De Kruif 1980)
44.83, 44.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.187 (mp at $99.24^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
1.65 (shake flask-nephelometry, Davis \& Parker 1942)
$1.60 \quad\left(27^{\circ} \mathrm{C}\right.$, nephelometry, Davis et al. 1942)
0.994 (shake flask-UV, Andrews \& Keefer 1949)
1.60 (shake flask-UV, Klevens 1950)
1.18 (Pierotti et al. 1959)
0.71 (shake flask, binding to bovine serum albumin, Sahyun 1966)
1.60 (shake flask-UV/fluorescence, Barone et al. 1967)
$2.67 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
1.18* (shake flask-UV, measured range $24.6-73.4^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-3890 /(\mathrm{T} / \mathrm{K})+4.08 \times 10^{-4} \cdot[(\mathrm{~T} / \mathrm{K})-291.15]^{2}-27.9+0.0374 \cdot(\mathrm{~T} / \mathrm{K})$; temp range $24.6-73.4^{\circ} \mathrm{C}$
(shake flask-UV measurements, Wauchope \& Getzen 1972)
3.03, $2.85\left(20^{\circ} \mathrm{C}\right.$, HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)
1.21 (shake flask-UV, Vesala 1974)
1.07 (shake flask-GC, Eganhouse \& Calder 1976)
1.29 (shake flask-fluorescence, Mackay \& Shiu 1977)
1.002 (Rossi 1977; Neff 1979)
1.151* (shake flask-UV, measured range $8.4-31.8^{\circ} \mathrm{C}$, Schwarz 1977)
1.002* (generator column-HPLC/UV, measured range $4-29^{\circ} \mathrm{C}$, May et al. 1978, 1983)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=324.0+5.413 \cdot\left(\mathrm{t} /{ }^{\circ}\right)+0.8059 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0025 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $4-29^{\circ} \mathrm{C}$ (generator column-
HPLC/UV, May et al. 1978)
$0.955^{*} \quad\left(24.3^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range $4.0-29.9^{\circ} \mathrm{C}$, May 1980)
0.816 (quoted, Verschueren 1983)
1.0 (generator column-HPLC/UV, Wasik et al. 1983)
1.28 (average lit. value, Pearlman et al. 1984)
1.29 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
1.10* (generator column-HPLC/UV, measured range 4.6-25.3 ${ }^{\circ} \mathrm{C}$, Whitehouse 1984)
$1.69 \quad\left(29^{\circ} \mathrm{C}\right.$, shake flask-GC/FID, Stucki \& Alexander 1987)
0.0446 (vapor saturation-UV, Akiyoshi et al. 1987)
1.08 (generator column-HPLC, Billington et al. 1988)
1.10* (recommended, IUPAC Solubility Data Series, Shaw 1989)
1.0 (generator column-HPLC, Vadas et al. 1991)
1.03 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
0.823 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
1.20 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
$\log \mathrm{S}_{\mathrm{L}}(\mathrm{mol} / \mathrm{L})=0.930-861.6 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
$\ln x=-2.546051-4053 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$7773^{*} \quad\left(230^{\circ} \mathrm{C}\right.$, isoteniscope- Hg , measured range $230-340^{\circ} \mathrm{C}$, Nelson \& Senseman 1922)
$3626^{*} \quad\left(203.6^{\circ} \mathrm{C}\right.$, isoteniscope- Hg manometer, measured range $203.6-346.8^{\circ} \mathrm{C}$, Mortimer \& Murphy 1923) $\log (\mathrm{P} / \mathrm{mmHg})=7.771-2990 /(\mathrm{T} / \mathrm{K}) ;$ temp range $203.6-346.8^{\circ} \mathrm{C}$ (Antoine eq., static isoteniscope method, Mortimer \& Murphy 1923)
133.3* (118.2 ${ }^{\circ} \mathrm{C}$, summary of literature data, temp range $118.2-340.2^{\circ} \mathrm{C}$, Stull 1947)
0.0997 (effusion method, Inokuchi et al. 1952)
0.0227* (effusion method, Bradley \& Cleasby 1953)
$\log (\mathrm{P} / \mathrm{cmHg})=10.388-4519 /(\mathrm{T} / \mathrm{K})$; temp range $36.7-49.65^{\circ} \mathrm{C}$ (Antoine eq., Bradley \& Cleasby 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=16.0-5008 /(\mathrm{T} / \mathrm{K})$; temp range $0-60^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958)
0.464 (extrapolated from Antoine eq. of liquid state $\mathrm{P}_{\mathrm{L}}$, Weast 1972-73)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 14184.0 /(\mathrm{T} / \mathrm{K})]+7.936781$; temp range $118.2-340^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
0.159 (extrapolated from Antoine eq. of liquid state $\mathrm{P}_{\mathrm{L}}$, Boublik et al. 1973)
30.4* $\quad\left(100.0^{\circ} \mathrm{C}\right.$, inclined-piston manometry, measured range $100.0-150.0^{\circ} \mathrm{C}$, Osborn \& Douslin 1975)
0.0187 (lit. average-interpolated, API 1979)
0.0263* (gas saturation, Macknick \& Prausnitz 1979)
0.0267 (extrapolated-Clapeyron eq., Macknick \& Prausnitz 1979)
$\log (\mathrm{P} / \mathrm{mmHg})=26.648-10484 /(\mathrm{T} / \mathrm{K})$; temp range $51.6-90.3^{\circ} \mathrm{C}$ (Clapeyron eq., gas saturation, Macknick \& Prausnitz 1979)
0.018* (effusion, De Kruif 1980)
$0.0161^{*} \quad$ (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=14.852-4962.77 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., Sonnefeld et al. 1983)
0.016 (generator column-HPLC/UV, Wasik et al. 1983)
$0.111,0.0688$ ( $\mathrm{P}_{\mathrm{GC}}$ by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
0.134 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ converted from literature $\mathrm{P}_{\mathrm{S}}$, Bidleman 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.61335-2593.134 /\left(224.402+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $203.6-346.8^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.01392-2039.351 /\left(168.569+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $230-340^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=7.26082-2379.04 /\left(203.76+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $176-379^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985,1992$)$
0.070 (Yamasaki et al. 1984)
0.0149 (selected, Howard et al. 1986)
0.012* (gas saturation, extrapolated-Antoine eq. from exptl. data, temp range $49-74^{\circ} \mathrm{C}$, Sato et al. 1986) $\ln (\mathrm{P} / \mathrm{Pa})=20.3950-2931.20 /(\mathrm{T} / \mathrm{K}-139.743)$; temp range: $322.9-347.8 \mathrm{~K}$ (Antoine eq., gas saturation, Sato et al. 1986)
0.025 (interpolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.305-4444 /(\mathrm{T} / \mathrm{K})$; temp range $296-315 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.70162-4554.38 /(\mathrm{T} / \mathrm{K})$; temp range $313-363 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.64812-2513.134 /(-65.345+\mathrm{T} / \mathrm{K})$; temp range $373-423 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.17186-3235.19 /(12.908+\mathrm{T} / \mathrm{K})$; temp range $391-613 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
0.0127, 0.0827 (literature mean $\mathrm{P}_{\mathrm{S}}$, supercooled liquid $\mathrm{P}_{\mathrm{L}}$, Bidleman \& Foreman 1987)
$0.111,0.0556 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$, GC-RT correlation with different reference standards, Hinckley et al. 1990)
$0.134,0.10$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ converted from literature $\mathrm{P}_{\mathrm{S}}$ with different $\Delta \mathrm{S}_{\text {fus }}$ values, Hinckley et al. 1990)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=11.46-3716 /(\mathrm{T} / \mathrm{K})(\mathrm{GC}-\mathrm{RT}$ correlation, Hinckley et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=50.2858-5.7409 \times 10^{3} /(\mathrm{T} / \mathrm{K})-13.935 \cdot \log (\mathrm{~T} / \mathrm{K})-8.852 \times 10^{-10} \cdot(\mathrm{~T} / \mathrm{K})+2.11343 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range $372-869 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
0.0708 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$0.0251,0.0227,0.018,0.0186 ; 0.0267,0.0161$ (quoted exptl.: effusion method, gas saturation, Delle Site 1997)
$0.0288,0.0227,0.0181 ; 0.0196,0.0122,0.0173$ (quoted lit.: calculated; from GC-RT correlation, Delle Site 1997)
0.0197* (Knudsen effusion/thermogravimetry technique, extrapolated Clausius-Clapeyron eq., Oja \& Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=34.387-11423 /(\mathrm{T} / \mathrm{K})$; temp range: $303-333 \mathrm{~K}$ (Clausius-Clapeyron eq., Knudsen effusion, Oja \& Suuberg 1998)
0.115; 0.0306 (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.38-3842 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.07-2982 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$0.0163 \pm 0.004$ (gas saturation-HPLC/fluorescence; de Seze et al. 2000)
$\log (\mathrm{P} / \mathrm{Pa})=14.852-4962.77 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
$0.0799 ; 0.0475$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3768 /(\mathrm{T} / \mathrm{K})+11.54 ; \Delta \mathrm{H}_{\text {vap }} .=-72.2 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
0.0202 (solid $\mathrm{P}_{\mathrm{S}}$, gas saturation-GC/MS, Mader \& Pankow 2003)
0.0966 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from $\mathrm{P}_{\mathrm{S}}$ assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Mader \& Pankow 2003)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
5.55 (gas stripping-GC, Southworth 1979)
3.981 (gas stripping-GC, Mackay et al. 1979; Mackay \& Shiu 1981; Mackay et al. 1982)
3.65 (gas stripping-GC, Mackay \& Shiu 1981; Mackay et al. 1982)
2.38 (wetted-wall column-GC, Fendinger \& Glotfelty 1990; quoted, Shiu \& Mackay 1997; Shiu et al. 1999)
3.97 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
4.68* (gas stripping-GC, measured range $5.9-34.7^{\circ} \mathrm{C}$, Alaee et al. 1996)
$\ln \mathrm{K}_{\mathrm{AW}}=6.0314-3524.18 /(\mathrm{T} / \mathrm{K})$; temp range $5.9-34.7^{\circ} \mathrm{C}$ (gas stripping-GC, Alaee et al. 1996)
3.61 (gas stripping-GC, Shiu \& Mackay 1997)
2.90 (gas stripping-HPLC/fluo., De Maagd et al. 1998)
4.29* (gas stripping-GC; measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-5689.2 /(\mathrm{T} / \mathrm{K})+12.75, \Delta \mathrm{H}=47.3 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left(\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right)=8.14-2120 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
$3.85 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=2.417-1530 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
4.46 (Hansch \& Fujita 1964; Leo et al. 1971; Hansch et al. 1973; Hansch \& Leo 1979)
4.66 (calculated-molecular connectivity indices MCI, Kier et al. 1971)
4.67 (calculated-fragment const., Rekker 1977)
4.57 (shake flask-UV, concn ratio, Karickhoff et al. 1979)
4.45 (HPLC-k' correlation, McDuffie 1981)
4.63 (RP-TLC-k' correlation, Bruggeman et al. 1982)
4.53 (HPLC-k' correlation, Hammers et al. 1982)
4.52; 4.31 (shake flask; HPLC correlation, Eadsforth \& Moser 1983)
4.46 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
4.28 (HPLC-k' correlation, Haky \& Young 1984)
4.39 (RP-HPLC-RT correlation, Chin et al. 1986)
4.50 (HPLC-RT correlation, Wang et al. 1986)
4.56 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
$4.52 \pm 0.15$ (recommended, Sangster 1989, 1993)
$4.374 \pm 0.034,4.562 \pm 0.006$ (shake flask/slow stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)
4.30 (centrifugal partition chromatography, Berthod et al. 1992)
4.46 (shake flask-UV spectroscopy, pH 7.4 , Alcron et al. 1993)
4.46 (recommended, Hansch et al. 1995)
4.53, $4.83 \quad\left(26^{\circ} \mathrm{C}, 4^{\circ} \mathrm{C}\right.$, quoted, Piatt et al. 1996)
$4.48 \pm 0.19,4.54 \pm 0.61 \quad$ (HPLC-k' correlation: ODS column, Diol column, Helweg et al. 1997)
4.57, 4.49-4.64 (shake flask/slow stirring-HPLC/fluo., mean value, De Maagd et al. 1998)
4.60 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson \& Schrăder 1999)
4.50; 4.65, 4.52 (shake flask-SPME solid-phase micro-extraction; quoted lit. values, Paschke et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equation:
7.45 (calculated, Finizio et al. 1997)
7.57*; 7.41 (generator column-GC; calculated-conen ratio $\mathrm{C}_{\mathrm{o}} / \mathrm{C}_{\mathrm{A}}$, measured range $0-40^{\circ} \mathrm{C}$, Harner \& Bidleman 1998)
$\log \mathrm{K}_{\mathrm{OA}}=-5.62+3942 /(\mathrm{T} / \mathrm{K})$; temp range $0-40^{\circ} \mathrm{C}, \Delta \mathrm{H}_{\mathrm{OA}}=63.3 \mathrm{~kJ} / \mathrm{mol}$ (generator column-GC, Harner \& Bidleman 1998)
7.52 (calculated-S oct and vapor pressure P, Abraham et al. 2001)
7.88 (solid-phase microextraction SPME-GC, Treves et al. 2001)

Bioconcentration Factor, log BCF:

| 3.42 (fa | (fathead minnow, Carlson et al. 1978) |
| :---: | :---: |
| 2.51 (D | (Daphnia pulex, Southworth et al. 1978) |
| 2.57 (ki | (kinetic estimation, Southworth et al. 1978) |
| 3.80 (mix | (mixed microbial population, Steen \& Karickhoff 1981) |
| 4.28 (P. | (P. hoyi, Eadie et al. 1982) |
| 3.67 (mic | (microorganisms-water, Mabey et al. 1982) |
| 4.38, 4.03, 4.57(average, Selenastum capricornutum-dosed singly, dosed simultaneously, Casserly et al. 1983) |  |
| 3.25 (C | (Chlorella fusca; Geyer et al. 1984) |
| 2.51 (fis | (fish, Govers et al. 1984) |
| 2.97, 3.25, 3.25 | 3.25 (activated sludge, algae, fish, Freitag et al. 1985) |
| 4.18; 4.28 (P. | (P. hoyi of Lake Michigan interstitial waters; of high sediment study site, Landrum et al. 1985) |
| 2.51 (D | (Daphnia magna, Newsted \& Giesy 1987) |
| 3.21 | ( $10-20^{\circ} \mathrm{C}$, h. limbata, rate constant ratio $\mathrm{k}_{1} / \mathrm{k}_{2}$, Landrum \& Poore 1988) |
| 4.45; 3.77; 3.43 | 3.43 ( $4^{\circ} \mathrm{C}$, P. hoyi; S. heringianus; Mysis relicta, quoted, Landrum \& Poore 1988) |
| 0.756, 1.487 | (Polychaete sp, Capitella capitata, Bayona et al. 1991) |

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
4.36 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
4.08 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
4.60 (fluorescence quenching interaction with AB humic acid, Gauthier et al. 1986)
4.28 (sediment from Tamar estuary, batch equilibrium-GC, Vowles \& Mantoura 1987)
4.00 (Aldrich and Fluka humic acids, Chin et al. 1989)
6.12 (sediments average, Kayal \& Connell 1990)
4.22, 4.28 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo 1990b)
4.42 (sandy surface soil, batch equilibrium-sorption isotherm, Wood et al. 1990)
4.07 (Quarry dark sand, batch equilibrium-sorption isotherm, Magee et al. 1991)
4.64 (DOM derived from soil, fluorescence quenching method, Magee et al. 1991)
4.42, 4.30 (marine porewater organic colloids; marine sediment, Fort Point Channel FPC 25-29 cm, Chin \& Gschwend 1992)
4.17; 4.18, 4.17 (sediment: concn ratio $\mathrm{C}_{\text {sed }} / \mathrm{C}_{\mathrm{w}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter \& Alden 1994)
4.50 (Rotterdam Harbor sediment $4.6 \%$ OC, batch sorption equilibrium, Hegeman et al. 1995)
4.37 (Speyer soil $1.08 \%$ OC, batch sorption equilibrium, Ou et al. 1995)
6.07, 7.03, 6.39; 4.12 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island; quoted lit., McGroddy \& Farrington 1995)
5.77 (marine sediments: Fort Point Channel FPC 25-29 cm, McGroddy \& Farrington 1995)
4.28, 4.12, 4.23 (RP-HPLC-k' correlation on different stationary phases, Szabo et al. 1995)
4.09; 4.32 (HPLC-screening method; calculated-PCKOC fragment method, Müller \& Kördel 1996)
4.18 (range $4.13-4.20)$; 3.56 (range $3.54-3.56)\left(4^{\circ} \mathrm{C}\right.$, low organic carbon sediment $\mathrm{f}_{\mathrm{OC}}=0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
4.13 (range 4.06-4.19); 3.48 (range 3.47-3.48) $\left(26^{\circ} \mathrm{C}\right.$, low organic carbon sediment $\mathrm{f}_{\mathrm{OC}}=0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
4.65; $4.81 \pm 0.16 \quad$ (humic acid, HPLC- $\mathrm{k}^{\prime}$ correlation; quoted lit., Nielsen et al. 1997)
2.42-2.56 (5 soils, $20^{\circ} \mathrm{C}$, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
4.27, 4.27, 4.12, 4.27, 4.10; mean $4.12 \pm 0.088$ (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choiu et al. 1998)
4.38, 4.45, 4.53, 4.33, 4.42, 4.62, $4.64 \pm 0.087$ (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLCfluorescence, Choiu et al. 1998)
$4.48 \quad(4.46-4.50), 4.22$ (4.20-4.23) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flaskHPLC/UV, de Maagd et al. 1998)
3.67; 3.29, 4.04, 3.27, 4.37, 4.21 (calculated-K ${ }_{\text {ow }}$; HPLC-screening method with different LC-columns, Szabo et al. 1999)
4.31-6.02 (range, calculated from sequential desorption of 11 urban soils; Krauss \& Wilcke 2001)
$5.34 ; 5.23,4.82,4.98\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)
4.39 - algae, 4.66 - degraded algae, 3.33 - cellulose, 4.72 - collagen, 4.50 - cuticle, 4.18 - lignin, 4.67 - humic acid, 4.56 - oxidized humic acid, 4.64 - Green River kerogen, 4.88 - Pula kerogen (aliphatic-rich sedimentary organic matter, batch experiments, Salloum et al. 2002)
4.28 (Askov soil - a Danish agricultural soil, Sverdrup et al. 2000)
4.03, 4.08 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%$, $\mathrm{OC} \geq 0.5 \%$, average, Delle Site 2001)
$4.34 \quad$ (average values for sediment OC $\geq 0.5 \%$, Delle Site 2001)
4.70 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)
4.66-4.90 (sediment/water, initial-final values of 5-100 d contact time, gas-purge technique-HPLC/fluo., ten Hulscher et al. 2003)
5.29-5.92, 5.98 (NIST SRM diesel particulate matter: flocculation-based batch equilibrium method with 59-d equilibration time, air-bridge equilibrium with 123-d equilibration time, Nguyen et al. 2004)
$4.30-5.3,5.2-5.5$ (sediments of 5 lakes with OC ranges from $0.12-21.03 \%$, solute concn at $1 \mathrm{mg} / \mathrm{L}$, at $1 \mathrm{ng} / \mathrm{L}$, sorption isotherms, Cornelissen et al. 2004)
4.80, 4.80, 4.50, 4.84 (sediment free of BC "black carbon": Lake Varparanta OC $0.12 \%$, Lake Kuorinka OC $1.39 \%$, Lake Höytiäinen OC $3.3 \%$, Lake Ketelmeer OC $5.51 \%$, equilibrium sorption isotherm, Cornelissen et al. 2004)

Environmental Fate Rate Constants, $k$, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: half-lives from solution: 97, 108 min (exptl., calculated, Mackay et al. 1983).
Photolysis: calculated $\mathrm{t}_{1 / 2}=8.4 \mathrm{~h}$ for direct sunlight photolysis at $40^{\circ} \mathrm{N}$ latitude of midday in midsummer, near surface water and $t_{1 / 2}=59 \mathrm{~d}$ (inland water) and $t_{1 / 2}=69 \mathrm{~d}$ for inland water with sediment partitioning in a 5-m deep inland water body (Zepp \& Schlotzhauer 1979)
$\mathrm{t}_{1 / 2}=3 \mathrm{~h}$, atmospheric and aqueous half-life, based on measured aqueous photolysis quantum yields and calculated for midday summer sunlight at $40^{\circ} \mathrm{N}$ latitude and $\mathrm{t}_{1 / 2}=25 \mathrm{~h}$ after adjusting for approximate winter sunlight intensity (Howard et al. 1991);
half-lives on different atmospheric particulate substrates (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=150 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=45 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=49 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985);
$\mathrm{t}_{1 / 2}=59 \mathrm{~d}$ under sunlight (Mill \& Mabey 1985);
$\mathrm{k}=0.11 \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=6.3 \mathrm{~h}$ in distilled water (Fukuda et al. 1988);
photodegradation $\mathrm{k}=6.53 \times 10^{-3} \mathrm{~min}$ and $\mathrm{t}_{1 / 2}=1.78 \mathrm{~h}$ in methanol-water $(2: 3, \mathrm{v} / \mathrm{v})$ solution with an initial concn of 5.0 ppm under high pressure mercury lamp or sunlight (Wang et al. 1991)
$\mathrm{k}($ expt $)=0.00653 \mathrm{~min}^{-1}$ pseudo-first-order direct photolysis rate constant with the calculated $\mathrm{t}_{1 / 2}=1.78 \mathrm{~h}$ and the predicted $\mathrm{k}=0.00165 \mathrm{~min}^{-1}$ calculated by QSPR, in aqueous solution when irradiated with a 500-W medium pressure mercury lamp (Chen et al. 1996);
direct photolysis $\mathrm{t}_{1 / 2}=4.62 \mathrm{~h}$ (observed), $\mathrm{t}_{1 / 2}=3.89 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001);
photochemical degradation under atmospheric conditions: $\mathrm{k}=(4.49 \pm 0.68) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(4.29 \pm 0.57) \mathrm{h}$ in diesel particulate matter, $\mathrm{k}=(2.11 \pm 0.04) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(9.1 \pm 0.19) \mathrm{h}$ in diesel particulate matter/soil mixture, and $\mathrm{t}_{1 / 2}=17-4.97 \mathrm{~h}$ in various soil components using a $900-\mathrm{W}$ photo-irradiator as light source; $\mathrm{k}=(3.17 \pm 0.06) \times 10^{-6} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(60.63 \pm 1.33) \mathrm{h}$ in diesel particulate matter using a $300-$ W light source (Matsuzawa et al. 2001)
Photodegradation $\mathrm{k}=0.09 \times 10^{-4} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, * data at other temperatures see reference:
k (aquatic fate rate) $=0.01 \mathrm{~L} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=8 \times 10^{6} \mathrm{~d}$ (Callahan et al. 1979)
k (calc) $<360 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}<36 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}=(1.33-1.57) \times 10^{4} \mathrm{dm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ over the pH range $1-7$ for the reaction with $\mathrm{O}_{3}$ in water at $25^{\circ} \mathrm{C}, \mathrm{t}_{1 / 2}=$ 0.44 s in presence of $10^{-4} \mathrm{M}$ ozone at pH 7 (Butković et al. 1983)
$\mathrm{k}_{\mathrm{OH}}=3.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $298 \pm 1 \mathrm{~K}, \mathrm{k}_{\mathrm{OH}}=2.8 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $319 \pm 1 \mathrm{~K}$ (relative rate method, Biermann et al. 1985)
$\mathrm{k}_{\mathrm{OH}} *=3.4 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K (review, Atkinson 1989)
$\mathrm{k}_{\mathrm{OH}}=25.7 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=27 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $346-386 \mathrm{~K}$ with a calculated atmospheric lifetime of 11 h based on gas-phase OH reactions (Brubaker \& Hites 1998)
Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation: $100 \%$ degradation within 7 d for a domestic sewage of an average of three static-flask screening test (Tabak et al. 1981);
$\mathrm{t}_{1 / 2}($ aerobic $)=384-4800 \mathrm{~h}$, based on aerobic soil die-away test data (Coover \& Sims 1987; quoted, Howard et al. 1991);
$\mathrm{k}=0.0447 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=16 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0196 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=35 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990);
$\mathrm{t}_{1 / 2}($ anaerobic $)=1536-19200 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$t_{1 / 2}=4 \mathrm{~d}$ in inorganic solution and $t_{1 / 2}=11 \mathrm{~d}$ in Kendaia soil (Manilal \& Alexander 1991)
removal rate of 1.10 and 0.12 mg ( g of volatile suspended solid d$)^{-1}$, degradation by bacteria from creosotecontaminated marine sediments with nitrate- and sulfate-reducers respectively under anaerobic conditions in a fluidized bed reactor (Rockne \& Strand 1998)
first-order $\mathrm{k}=0.033$ to $0.139 \mathrm{~L} \mathrm{mg}^{-1} \mathrm{~d}^{-1}$ for a marine PAH-degrading enrichment without sediment, the degradation rate was 2.1 to 3.5 times faster with sediment present (Poeton et al. 1999)
Biotransformation: for bacteria, $1.6 \times 10^{-7} \mathrm{~mL}$ cell ${ }^{-1} \mathrm{~h}^{-1}$ (Paris et al. 1980; quoted, Mabey et al. 1982)
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
$\mathrm{k}_{1}=203 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.543 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)
$\log \mathrm{k}_{1}=2.31 \mathrm{~h}^{-1} ; \log \mathrm{k}_{2}=-0.27 \mathrm{~h}^{-1}$ (Daphnia pulex, as per the correlation of Mackay \& Hughes 1984, Hawker \& Connell 1986)
$\mathrm{k}_{1}=129.0 \mathrm{~mL} \mathrm{~g} \mathrm{~g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0046 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, $p$. hoyi, Landrum 1988; quoted, Landrum \& Poore 1988)
$\mathrm{k}_{1}=52.5 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.032 \mathrm{~h}^{-1}\left(10-20^{\circ} \mathrm{C}\right.$, H. limbata, Landrum \& Poore 1988)
$\mathrm{k}_{1}=94.0 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.016 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, S. heringianus, quoted, Landrum \& Poore 1988)
$\mathrm{k}_{1}=32.0 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.012 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, Mysis relicta, quoted, Landrum \& Poore 1988)
$\mathrm{k}_{1}=8.8 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.045 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $t_{1 / 2}=6 \mathrm{~h}$ with a steady-state concn of tropospheric ozone of $2 \times 10^{-9} \mathrm{M}$ in clean air (Butković et al. 1983) $t_{1 / 2}=2.01-20.1 \mathrm{~h}$, based on photooxidation half-life in air (Howard et al. 1991); calculated atmospheric lifetime of 11 h based on gas-phase OH reactions (Brubaker \& Hites 1998).
Surface water: computed near-surface of a water body, $t_{1 / 2}=8.4 \mathrm{~h}$ for direct photochemical transformation at latitude $40^{\circ} \mathrm{N}$, midday, midsummer with $\mathrm{t}_{1 / 2}=59 \mathrm{~d}$ (no sediment-water partitioning), $\mathrm{t}_{1 / 2}=69 \mathrm{~d}$ (with sedimentwater partitioning) on direct photolysis in a 5-m deep inland water body (Zepp \& Schlotzhauer 1979); $\mathrm{t}_{1 / 2}=0.44 \mathrm{~s}$ in presence of $10^{-4} \mathrm{M}$ ozone at pH 7 (Butković et al. 1983); calculated $t_{1 / 2}=59 \mathrm{~d}$ under sunlight for summer at $40^{\circ} \mathrm{N}$ latitude (Mill \& Mabey 1985); $\mathrm{t}_{1 / 2}=3-25 \mathrm{~h}$, based on aqueous photolysis half-life (Howard et al. 1991); photolysis $\mathrm{t}_{1 / 2}=1.78 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater: $t_{1 / 2}=768-9600 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: reduction $\mathrm{t}_{1 / 2}($ est. $)=1196 \mathrm{~h}, \mathrm{t}_{1 / 2}(\operatorname{exptl})=825 \mathrm{~h}$ for chemical available phenanthrene and $\mathrm{t}_{1 / 2}=151 \mathrm{~h}$ for bioavailable phenanthrene for amphipod, $P$. hoyi in Lake Michigan sediments at $4^{\circ} \mathrm{C}$. The average uptake clearance from sediment was $(0.041 \pm 0.023) \mathrm{g}$ of dry sediment $\cdot \mathrm{g}^{-1}$ of organism $\cdot \mathrm{h}^{-1}$, and the rate constants to become biologically unavailable was $(0.0055 \pm 0.003) \mathrm{h}^{-1}$ resulting a bioavailable $\mathrm{t}_{1 / 2}=126 \mathrm{~h}$ (Landrum 1989); desorption $\mathrm{t}_{1 / 2}=8.6 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $\mathrm{t}_{1 / 2}=2.5-26 \mathrm{~d}$ (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$\mathrm{t}_{1 / 2}=9.7 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and $\mathrm{t}_{1 / 2}=14 \mathrm{~d}$ for $50 \mathrm{mg} / \mathrm{kg}$ (Bulman et al. 1987);
biodegradation $\mathrm{k}=0.0447 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=16 \mathrm{~d}$ in Kidman sandy loam soil and $\mathrm{k}=0.0196 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=35 \mathrm{~d}$ in McLaurin sandy loam soil (Park et al. 1990);
biodegradation $\mathrm{t}_{1 / 2}=11 \mathrm{~d}$ in Kendaia soil (Manilal \& Alexander 1991);
$\mathrm{t}_{1 / 2}=384-4800 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991);
$t_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
$\mathrm{t}_{1 / 2}=0.4-26 \mathrm{wk}, 5.7 \mathrm{yr}$ (quoted, Luddington soil, Wild et al. 1991).
Biota: depuration $\mathrm{t}_{1 / 2}=40.9 \mathrm{~h}$ in $S$. heringianus (Frank et al. 1986);
elimination $\mathrm{t}_{1 / 2}=9 \mathrm{~d}$ from rainbow trout, $\mathrm{t}_{1 / 2}=8.4 \mathrm{~d}$ from clam Mya arenaria, $\mathrm{t}_{1 / 2}=1.9 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=7 \mathrm{~d}$ from polychaete Abarenicola pacifica, $\mathrm{t}_{1 / 2}=3.4 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=0.9 \mathrm{~d}$ from shrimp, $t_{1 / 2}=4.8 \mathrm{~d}$ from polychaete Nereis virens, $\mathrm{t}_{1 / 2}=6.1 \mathrm{~d}$ from clam Mercenario mercenaria (Meador et al. 1995).

TABLE 4.1.1.23.1
Reported aqueous solubilities of phenanthrene at various temperatures
1.

| Wauchope \& Getzen 1972 |  |  |  | Schwarz 1977 |  | May et al. 1978a |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  |  |  | shake flask-fluorescence |  | generator column-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathbf{m}^{-3}$ |
|  | experimental |  | smoothed |  |  |  |  |
| 24.6 | 1.12 | 0 | 0.39 | 8.4 | 0.501 | 8.5 | 0.423 |
| 24.6 | 1.11 | 24.8 | 1.16 | 11.1 | 0.5507 | 10.0 | 0.468 |
| 29.9 | 1.49 | 25 | 1.18 | 14.0 | 0.640 | 12.5 | 0.512 |
| 29.9 | 1.49 | 29.9 | 1.49 | 17.5 | 0.784 | 15.0 | 0.601 |
| 30.3 | 1.47 | 30.3 | 1.52 | 20.2 | 0.881 | 21.0 | 0.816 |
| 30.3 | 1.48 | 38.4 | 2.27 | 23.3 | 1.085 | 24.3 | 0.995 |
| 38.4 | 2.44, 2.45 | 40.1 | 2.47 | 25.0 | 1.151 | 29.9 | 1.277 |
| 40.1 | 2.27, 2.28 | 47.5 | 3.63 | 29.3 | 1.372 |  |  |
| 40.1 | 2.25 | 50 | 4.14 | 34.6 | 1.627 | temp | ce eq. 2 |
| 47.5 | 3.87, 3.88 | 50.1 | 4.16 |  |  | S | $\mu \mathrm{g} / \mathrm{kg}$ |
| 47.5 | 3.87 | 50.2 | 4.19 | $\Delta \mathrm{H}_{\text {sol }} /$ / k | $)=36.32$ | a | 0.0025 |
| 50.1 | 4.30, 4.38 | 54.7 | 5.34 |  |  | b | 0.8059 |
| 50.1 | 4.32 | 59.2 | 6.85 |  |  | c | 5.413 |
| 50.2 | 4.08, 4.04 | 60.5 | 7.30 |  |  | d | 324 |
| 50.2 | 4.11 | 65.1 | 9.60 |  |  |  |  |
| 54.7 | 5.66, 5.64 | 70.7 | 13.3 |  |  |  |  |
| 54.7 | 5.63 | 71.9 | 14.2 |  |  | May | 978b |
| 59.2 | 7.17, 7.19 | 73.4 | 15.6 |  |  | generat | mn-HPLC |
| 59.2 | 7.21 | 75 | 17.2 |  |  | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 60.5 | 7.20, 7.60 |  |  |  |  |  |  |
| 65.1 | 9.80 | temp depe | ce eq. 1 |  |  | 25 | 1.002 |
| 65.1 | 9.70 | $\ln x$ | mole fraction |  |  | 29 | 1.220 |
| 65.1 | 9.80 | $\Delta \mathrm{H}_{\text {fus }}$ | $16.28 \pm 0.08$ |  |  |  |  |
| 70.7 | 12.4 | $10^{2} \cdot \mathrm{~b}$ | $3.74 \pm 0.13$ |  |  | temp | ce eq. 2 |
| 70.7 | 12.6 | c | $27.9 \pm 0.4$ |  |  | S | $\mu \mathrm{g} / \mathrm{kg}$ |
| 70.7 | 12.4 |  |  |  |  | a | 0.0025 |
| 71.9 | 18.8 |  |  |  |  | b | 0.8059 |
| 73.4 | 21.5 |  |  |  |  | c | 5.413 |
|  |  |  |  |  |  | d | 324 |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=16.28$ |  |  |  |  |  |  |  |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\text {sol }} /$ <br> for ten | $\begin{gathered} =34.81 \\ 5-30^{\circ} \mathrm{C} \end{gathered}$ |

Empirical temperature dependence equations:
Wauchope \& Getzen (1972): R•ln $x=-\left[\mathrm{H}_{\text {fus }} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{T} / \mathrm{K})$
(1)

May et al. (1978):-S/( $\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}_{1 / 2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}$

TABLE 4.1.1.23.1 (Continued)
2.

| May 1980 |  |  | 1983 | Whitehouse 1984 <br> generator columnHPLC/UV |  | Shaw 1989 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| generator column-HPLC |  | generator column-HPLC |  |  |  | IUPAC recommended |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 4.0 | 0.361 | 4.0 | 0.361 | 4.6 | 0.358 | 0 | 0.40 |
| 8.5 | 0.423 | 8.5 | 0.423 | 8.8 | 0.437 | 10 | 0.50 |
| 10 | 0.468 | 10.0 | 0.468 | 12.9 | 0.556 | 20 | 0.85 |
| 12.5 | 0.512 | 12.5 | 0.512 | 17.0 | 0.720 | 25 | 1.10 |
| 15 | 0.601 | 15.5 | 0.602 | 21.1 | 0.880 | 30 | 1.40 |
| 20 | 0.787 | 20.0 | 0.788 | 25.3 | 1.10 | 40 | 2.50 |
| 21 | 0.816 | 21.0 | 0.817 |  |  | 50 | 4.10 |
| 24.3 | 0.955 | 24.3 | 0.956 |  |  | 50 | 7.20 |
| 1.227  1.988 75 |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |

temp dependence eq. 2

| S | $\mu \mathrm{g} / \mathrm{kg}$ |
| :---: | :---: |
| a | 0.0025 |
| b | 0.8059 |
| c | 5.412 |
| d | 324 |

$\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=34.81$
for temp range $5-30^{\circ} \mathrm{C}$


FIGURE 4.1.1.23.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for phenanthrene.

TABLE 4.1.1.23.2
Reported vapor pressures of phenanthrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
1.

| Nelson \& Senseman 1922 |  | Mortimer \& Murphy 1923 |  | Stull 1947 |  | Bradley \& Cleasby 1953 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| isoteniscope-Hg manometer |  | isoteniscope-Hg manometer |  | summary of literature data |  | effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 230 | 7773 | 203.6 | 3626 | 118.2 | 133.3 | 36.7 | 0.0853 |
| 235 | 9079 | 233.8 | 8999 | 154.3 | 666.6 | 39.85 | 0.1187 |
| 240 | 10532 | 246.0 | 12572 | 173.0 | 1333 | 42.0 | 0.160 |
| 245 | 12146 | 271.5 | 24265 | 193.7 | 2666 | 46.7 | 0.2466 |
| 250 | 13919 | 271.5 | 24398 | 215.8 | 5333 | 48.8 | 0.2973 |
| 255 | 15892 | 293.1 | 39957 | 229.0 | 7999 | 48.8 | 0.3000 |
| 260 | 18065 | 293.2 | 39970 | 249.0 | 13332 | 39.15 | 0.1080 |
| 265 | 20492 | 293.2 | 39983 | 277.1 | 26664 | 42.1 | 0.1480 |
| 270 | 23145 | 306.4 | 53222 | 308.0 | 53329 | 44.62 | 0.1933 |
| 275 | 26091 | 324.5 | 53289 | 340.2 | 101325 | 46.7 | 0.2426 |
| 280 | 18331 | 324.9 | 77954 |  |  | 49.65 | 0.3213 |
| 285 | 32891 | 325.4 | 78487 | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | 99.5 |  |  |
| 290 | 36810 | 337.1 | 79007 |  |  | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
| 300 | 45823 | 337.1 | 98792 |  |  | A | 10.388 |
| 310 | 56529 | 345.1 | 115244 |  |  | B | 4519 |
| 320 | 69169 | 245.7 | 116110 |  |  |  |  |
| 330 | 83913 | 346.8 | 117844 |  |  |  |  |
| 340 | 100925 |  |  |  |  |  |  |

2. 



TABLE 4.1.1.23.2 (Continued)

| Hoyer \& Peperle 1958 |  | Osborn \& Douslin 1975 |  | Macknick \& Prausnitx 1979 |  | de Kruif 1980 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| effusion |  | inclined-piston manometry |  | gas saturation-GC |  | effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\prime} \mathrm{C}$ | P/Pa | $t^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  |  | $\Delta \mathrm{H}_{\mathrm{v}} /(\mathrm{kJ} \mathrm{m}$ at 398.15 at tp | $\begin{aligned} & 68.58 \\ & 70.79 \end{aligned}$ |  |  |  |  |
|  |  | $\begin{aligned} & \Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=87.24 \\ & \quad \text { at tp } \end{aligned}$ |  |  |  |  |  |
|  |  | $\Delta \mathrm{f}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=16.44$ |  |  |  |  |  |

3. 


$\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=95.0$


FIGURE 4.1.1.23.2 Logarithm of vapor pressure versus reciprocal temperature for phenanthrene.

TABLE 4.1.1.23.3
Reported Henry's law constants and octanol-air partition coefficients of phenanthrene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$
(1a)

Henry's law constant



FIGURE 4.1.1.23.3 Logarithm of Henry's law constant and $K_{O A}$ versus reciprocal temperature for phenanthrene.

### 4.1.1.24 1-Methylphenanthrene



Common Name: 1-Methylphenanthrene
Synonym:
Chemical Name: 1-methylphenanthrene
CAS Registry No: 832-69-6
Molecular Formula: $\mathrm{C}_{15} \mathrm{H}_{12}$
Molecular Weight: 192.256
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
123 (Weast 1982-83; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
354 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$188.0 \quad$ (Ruelle \& Kesselring 1997)
221.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.109\left(\mathrm{mp}\right.$ at $\left.123^{\circ} \mathrm{C}\right)$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated. Additional data at other temperatures designated ${ }^{*}$, are compiled at the end of this section):
$0.255^{*} \quad\left(24.1^{\circ} \mathrm{C}\right.$, generator column-HPLC/UV, measured range $6.6-29.9^{\circ} \mathrm{C}$, May et al. $\left.1978 \mathrm{a}, 1983\right)$
0.269 (generator column-HPLC, May et al. 1978b)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=55.42+6.8016 \cdot\left(\mathrm{t} /{ }^{\circ}\right)-0.1301 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0080 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $6.6-29.9^{\circ} \mathrm{C}$ (generator columnHPLC/UV, May et al. 1978)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equation):
0.0186; 0.0160 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3987 /(\mathrm{T} / \mathrm{K})+11.64 ; \Delta \mathrm{H}_{\text {vap }} .=-76.3 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
5.0* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-4257.88 /(\mathrm{T} / \mathrm{K})+8.0587, \Delta \mathrm{H}=35.4 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
5.08 (HPLC-RT correlation, Wang et al. 1986)
5.08 (recommended, Sangster 1989, 1994)
5.08 (recommended, Hansch et al. 1995)
5.10-5.20; 5.15 (quoted lit. range; lit. mean, Meador et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: photodegradation of 5 ppm initial concentration in methanol-water ( $3: 7 \mathrm{~h} \mathrm{v} / \mathrm{v}$ ) by high pressure mercury lamp or sunlight with a rate constant $\mathrm{k}=1.84 \times 10^{-3} \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=6.27 \mathrm{~h}$ (Wang et al. 1991); the
pseudo-first-order direct photolysis $\mathrm{k}(\operatorname{exptl})=0.00184 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=6.27 \mathrm{~h}$ and the predicted $\mathrm{k}=0.0026 \mathrm{~min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);
direct photolysis $t_{1 / 2}=3.10 \mathrm{~h}$ (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: direct photolysis $t_{1 / 2}=3.10 \mathrm{~h}$ (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).
Surface water: photolysis $t_{1 / 2}=6.27 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=6.7 \mathrm{~d}$ from Oyster, 6.0 d from clam Mercenario mercenaria (quoted, Meador et al. 1995).

## TABLE 4.1.1.24.1

Reported aqueous solubilities and Henry's law constant of 1-methylphenanthrene at various temperature and the empirical temperature dependence equations
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}$

| Aqueous solubility |  |  |  |  |  | Henry's law constant <br> Bamford et al. 1999 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| May et al. 1978a |  | May et al. 1978b |  | May 1980, 1983 |  |  |  |
| generator column-HPLC |  | generator column-HPLC |  | generator column-HPLC |  | gas stripping-GC/MS |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
| 6.6 | 0.0952 | 25.0 | 0.269 | 6.6 | 0.0952 | 4.1 | 1.42, 1.75 |
| 8.9 | 0.114 |  |  | 8.9 | 0.114 |  | av. 1.58 |
| 14.0 | 0.147 | temp d | ce eq. 1 | 14.0 | 0.147 | 11.0 | 2.20, 2.53 |
| 19.2 | 0.193 | S | $\mu \mathrm{g} / \mathrm{kg}$ | 19.2 | 0.193 |  | av. 2.36 |
| 24.1 | 0.255 | a | 0.0080 | 24.1 | 0.255 | 18.0 | 3.26, 3.69 |
| 26.9 | 0.304 | b | 0.1301 | 26.9 | 0.304 |  | av. 3.47 |
| 29.9 | 0.355 | c | 6.8016 | 29.9 | 0.355 | 25.0 | 4.62, 5.42 |
|  |  | d | 55.42 |  |  |  | av. 5.00 |
| data of May et al. 1978a |  | $\begin{gathered} \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=30.08 \\ \text { measured between } 5-30^{\circ} \mathrm{C} \end{gathered}$ |  | data of May 1980 fitted to temp dependence eq. 1 |  | 31.0 | 6.09, 7.52 |
|  |  |  | av. 6.77 |  |  |  |  |
| S | $\mu \mathrm{g} / \mathrm{kg}$ |  |  | S | $\mu \mathrm{g} / \mathrm{kg}$ |  |  |
| a | 0.0080 |  |  | a | 0.0074 | $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| b | 0.1301 |  |  | b | -0.0858 | A | 8.0587 |
| c | 6.8016 |  |  | c | 5.785 | B | 4257.88 |
| d | 55.42 |  |  | d | 62.9 |  |  |
|  |  |  |  |  |  |  |  | enthal $\Delta \mathrm{H} /(\mathrm{kJ}$ | ntropy change: $\left.{ }^{-1}\right)=35.4 \pm 1.9$ |
|  |  |  |  |  |  | $\Delta \mathrm{S} /$ | $\left.\mathrm{mol}^{-1}\right)=67$ |
|  |  |  |  |  |  |  | at $25^{\circ} \mathrm{C}$ |



FIGURE 4.1.1.24.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1-methylphenanthrene.

### 4.1.1.25 Anthracene



Common Name: Anthracene
Synonym: paranaphthalene, green oil, tetra olive NZG
Chemical Name: anthracene
CAS Registry No: 120-12-7
Molecular Formula: $\mathrm{C}_{14} \mathrm{H}_{10}$
Molecular Weight: 178.229
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
215.76 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
339.9 (Lide 2003)

Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.25 \quad\left(27^{\circ} \mathrm{C}\right.$, Dean 1985)
$1.28 \quad\left(25^{\circ} \mathrm{C}\right.$, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
139 (calculated-density, liquid molar volume, Lande \& Banerjee 1981)
196.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
28.83 (Parks \& Huffman 1931)
28.87 (Tsonopoulos \& Prausnitz 1971; Ruelle \& Kesselring 1997)
29.37 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
58.99 (Tsonopoulos \& Prausnitz 1971; Wauchope \& Getzen 1972; Ubbelohde 1978)
58.58 (Casellato et al. 1973)
55.65 (De Kruif 1980)
60.08, 44.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0134 ( mp at $215.76^{\circ} \mathrm{C}$ )
0.0101 (calculated, $\Delta \mathrm{S}_{\text {fus }}=58.6 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.075 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.075 (shake flask-UV, Klevens 1950)
0.075 (Pierotti et al. 1959; Weimer \& Prausnitz 1965)
0.112 (shake flask, binding to bovine serum albumin-UV, Sahyun 1966)
0.080 (shake flask-UV/fluorescence, Barone et al. 1967)
$0.043 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
0.040 (shake flask-UV, Eisenbrand \& Baumann 1970)
$0.171,0.0392\left(20^{\circ} \mathrm{C}\right.$, HPLC-relative retention correlation, different stationary or mobile phases, Locke 1974)
$0.075^{*} \quad$ (extrapolated value, shake flask-UV, measured range $25-74.7^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-6930 /(\mathrm{T} / \mathrm{K})+4.08 \times 10^{-4} \cdot[(\mathrm{~T} / \mathrm{K})-291.15]^{2}-19.3+0.0181 \cdot(\mathrm{~T} / \mathrm{K})$, temp range $35.4-73.4^{\circ} \mathrm{C}$ (shake flask-UV measurements, Wauchope \& Getzen 1972)
0.030 (fluorescence/UV, Schwarz \& Wasik 1976)
0.073 (shake flask-fluorescence, Mackay \& Shiu 1977)
$0.0446 \quad$ (Rossi 1977; Neff 1979)
0.041* (shake flask-UV, measured range $8.6-31.3^{\circ} \mathrm{C}$, Schwarz 1977)
0.074 (Lu et al. 1978)
$0.0446^{*} \quad$ (generator column-HPLC/UV, measured range $5.2-29.3^{\circ} \mathrm{C}$, May et al. 1978)
$0.0434^{*} \quad\left(24.6^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range $5.2-28.7^{\circ} \mathrm{C}$, May 1980)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=8.21+0.8861 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+0.0097 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0013 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $5.2-29.3^{\circ} \mathrm{C}$ (generator columnHPLC/UV, May et al. 1978)
$0.033 \quad\left(20^{\circ} \mathrm{C}\right.$, generator column-fluorescence, Hashimoto et al. 1982)
$0.0434^{*} \quad\left(24.6^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range $5.6-29.3^{\circ} \mathrm{C}$, May et al. 1983)
0.030, 0.051 (generator column-HPLC/UV, Swann et al. 1983)
$0.04257^{*}$ (generator column-spectrofluorimetry, measured range $10-30^{\circ} \mathrm{C}$, Velapoldi et al. 1983)
0.0446 (generator column-HPLC/UV, Wasik et al. 1983)
0.066 (average lit. value, Pearlman et al. 1984)
0.0698 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
$0.0442^{*} \quad$ (generator column-HPLC/UV, measured range $4.6-25.3^{\circ} \mathrm{C}$, Whitehouse 1984)
0.0446 (vapor saturation-UV, Akiyoshi et al. 1987)
0.0443, 0.034 (generator column-HPLC/UV, Billington et al. 1988)
$0.041 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask/UV, ring test, Kishi \& Hashimoto 1989)
0.062* (recommended, IUPAC Solubility Data Series, Shaw 1989)
$0.070 \quad\left(23^{\circ} \mathrm{C}\right.$, shake flask-HPLC/UV/fluorescence, Pinal et al. 1991)
0.058 (generator column-HPLC, Vadas et al. 1991)
0.0488 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)
0.043 (shake flask-HPLC, Haines \& Sandler 1996)
0.0796 ; $0.138,0.0743$ (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)
0.093 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
0.070 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=1.679-1509 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
$\ln x=-1.43611-5307.35 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
$0.0434^{*} \quad\left(24.61^{\circ} \mathrm{C}\right.$, generator column-HPLC/fluo., Reza et al. 2002)
$\ln x=(0.50 \pm 0.45)+[(-5876 \pm 135) /(\mathrm{T} / \mathrm{K})]$; temp range $282.09-323.07 \mathrm{~K}$ (Reza et al. 2002)
$0.0438^{*}$ (generator column-HPLC/UV, measured range $0-50^{\circ} \mathrm{C}$, Dohányosová et al. 2003)
$\ln x=-33.7547+14.5018 / \tau+\mathrm{C} \ln \tau, \tau=(\mathrm{T} / \mathrm{K}) / 298.15 \mathrm{~K}$; temp range $0-50^{\circ} \mathrm{C}$ (generator column-HPLC/UV, temp range $0-50^{\circ} \mathrm{C}$, Dohányosová et al. 2003)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
5680* $\quad\left(220^{\circ} \mathrm{C}\right.$, isoteniscope- Hg , measured range $220-342^{\circ} \mathrm{C}$, Nelson \& Senseman 1922)
$6399^{*} \quad\left(223.3^{\circ} \mathrm{C}\right.$, isoteniscope- Hg manometer, measured range $223.3-340.5^{\circ} \mathrm{C}$, Mortimer \& Murphy 1923) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=10.972-4595 /(\mathrm{T} / \mathrm{K})$; temp range $100-210^{\circ} \mathrm{C}$ (Antoine eq., static isoteniscope method, Mortimer \& Murphy 1923)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=7.910-3093 /(\mathrm{T} / \mathrm{K})$; temp range $223.2-340.5^{\circ} \mathrm{C}$ (Antoine eq., static isoteniscope method, Mortimer \& Murphy 1923)
$133.3^{*} \quad\left(145.0^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $145.0-342.0^{\circ} \mathrm{C}$, Stull 1947)
0.001014 (static method-Rodebush gauge, Sears \& Hopke 1949)
$\log (\mathrm{P} / \mathrm{mmHg})=12.0072-5102.6 /(\mathrm{T} / \mathrm{K})$; temp range $378-398 \mathrm{~K}$ (Rodebush gauge, Sears \& Hopke 1949)
$3.60 \times 10^{-3}$ (effusion method, Inokuchi et al. 1952; quoted, Bidleman 1984)
$8.31 \times 10^{-4 *}$ (effusion method, Bradley \& Cleasby 1953)
$\log (\mathrm{P} / \mathrm{cmHg})=11.638-5320 /(\mathrm{T} / \mathrm{K})$; temp range $65.7-80.4^{\circ} \mathrm{C}$ (Antoine eq., Bradley \& Cleasby 1953)
$1.04 \times 10^{-3} \quad$ (fluorescence spectroscopy, Stevens 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=12.002-5102 /(\mathrm{T} / \mathrm{K})$; temp range 396-421 K (fluorescence, Stevens 1953)
$\log (\mathrm{P} / \mathrm{mmHg})=11.15-5401 /(\mathrm{T} / \mathrm{K})$; temp range $30-100^{\circ} \mathrm{C}$, (Knudsen effusion method, Hoyer \& Peperle 1958) $8.62 \times 10^{-4}$ (effusion method, Kelley \& Rice 1964)
$\log (\mathrm{P} / \mathrm{mmHg})=12.068-5145 /(\mathrm{T} / \mathrm{K})$; temp range $69-86^{\circ} \mathrm{C}$ (effusion method, Kelley \& Rice 1964)
$3.87 \times 10^{-7} \quad$ (Wakayama \& Inokuchi 1967)
$0.0024^{*}$ (effusion method-interpolated, measured range 290.1-358 K, Wiedemann \& Vaughan 1969, Wiedemann 1972)
$\log (\mathrm{P} / \mathrm{mmHg})=10.0216-4397.60 /(\mathrm{T} / \mathrm{K})$; temp range 290.1-358 K (Knudsen method, Wiedemann \& Vaughan 1969, Wiedemann 1972)
$\log (\mathrm{P} / \mathrm{mmHg})=7.67401-2819.63 /\left(247.02+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $175.5-380^{\circ} \mathrm{C}$ (liquid state, Antoine eq., Zwolinski \& Wilhoit 1971)
$\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 16823.6 /(\mathrm{T} / \mathrm{K})]+8.70760$; temp range $100-600^{\circ} \mathrm{C}$ (Antoine eq., Weast $1972-73$ )
$1.113 \times 10^{-3 *} \quad$ (Knudsen effusion weight-loss method, extrapolated Malaspina et al. 1973)
$\log (\mathrm{P} /$ torr $)=12.616-5277 /(\mathrm{T} / \mathrm{K})$; temp range $352.7-432.3 \mathrm{~K}$ (Knudsen method, Malaspina et al. 1973)
$1.47 \times 10^{-5}$ (effusion method, Murray et al. 1974)
$0.026 \quad\left(20^{\circ} \mathrm{C}\right.$, Radding et al. 1976)
$9.04 \times 10^{-4} \quad$ (effusion method, Taylor \& Crooks 1976)
$5.59 \times 10^{-3} \quad$ (gas saturation, Power et al. 1977)
$1.41 \times 10^{-3 *}$ (gas saturation, extrapolated-Clapeyron eq., measured range $85.25-119.95^{\circ} \mathrm{C}$, Macknick \& Prausnitz 1979)
$\log (\mathrm{P} / \mathrm{mmHg})=26.805-11402 /(\mathrm{T} / \mathrm{K})$; temp range $85.25-119.95^{\circ} \mathrm{C}$ (Clapeyron eq., gas saturation, Macknick \& Prausnitz 1979)
$7.50 \times 10^{-4 *}$ (effusion methods, extrapolated, measured range $64.44-87.74^{\circ} \mathrm{C}$, De Kruif 1980)
$4.90 \times 10^{-4}$ (calculated-TSA, Amidon \& Anik 1981)
$1.83 \times 10^{-3 *}$ (gas saturation, extrapolated-Antoine eq., measured range $50-85^{\circ} \mathrm{C}$, Grayson \& Fosbraey 1982)
$1.44 \times 10^{-3 *}$ (gas saturation, extrapolated-Antoine eq. measured range $80-125^{\circ} \mathrm{C}$, Bender et al. 1983)
$\ln (\mathrm{P} / \mathrm{Pa})=31.620-11378 /(\mathrm{T} / \mathrm{K})$; temp range $353.6-398.6 \mathrm{~K}$ (Antoine eq., Bender et al. 1983)
$8.0 \times 10^{-4 *}$ (gas saturation-HPLC/fluo./UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=12.977-4791.87 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., Sonnefeld et al. 1983)
$8.0 \times 10^{-4} \quad$ (gas saturation-HPLC, Wasik et al. 1983)
$0.10,0.0638\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
0.0865 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with $\Delta \mathrm{S}_{\text {fus }}$ Bidleman 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.53182-2550.737 /\left(221.756+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $223.2-340.5^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.66266-2659.55 /\left(230.119+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.$ ); temp range $220-310^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=8.91-3761 /(\mathrm{T} / \mathrm{K})$; temp range: $100-160^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=7.67401-2819.63 /\left(247.02+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range: $176-380^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992) $1.06 \times 10^{-3 *}$ (gas saturation-GC, Rordorf 1985)
$8.05 \times 10^{-4 *}$ (extrapolated-Clausius-Clapeyron eq. on gas saturation data, Hansen \& Eckert 1986)
$\log (\mathrm{P} / \mathrm{mPa})=17.88-5359 /(\mathrm{T} / \mathrm{K})$; temp range $313-363 \mathrm{~K}$ (Clausius-Clapeyron eq., Hansen \& Eckert 1986)
$1.14 \times 10^{-3}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.58991-4903.3 /(-1.58+\mathrm{T} / \mathrm{K})$; temp range $299-439 \mathrm{~K}$ (solid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.76139-5315.532 /(\mathrm{T} / \mathrm{K})$; temp range $313-363 \mathrm{~K}$, (solid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.75544-4947.751 /(\mathrm{T} / \mathrm{K})$; temp range $363-393 \mathrm{~K}$ (solid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.47799-3612.44 /(-44.906+\mathrm{T} / \mathrm{K})$; temp range $504-615 \mathrm{~K}$ (liquid, Antoine eq.-IV, Stephenson \& Malanowski 1987)
$5.73 \times 10^{-4} ; 5.60 \times 10^{-3}$ (literature mean solid $\mathrm{P}_{\mathrm{S}}$, supercooled liquid $\mathrm{P}_{\mathrm{L}}$, Bidleman \& Foreman 1987)
$0.086,0.0940$ (supercooled $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with different $\Delta \mathrm{S}_{\text {fus }}$ values, Hinckley et al. 1990)
$0.100,0.0689$ ( $\mathrm{P}_{\mathrm{GC}}$ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log \mathrm{P}_{\mathrm{L}} / \mathrm{Pa}=11.18-3642 /(\mathrm{T} / \mathrm{K})(\mathrm{GC}-\mathrm{RT}$ correlation, Hinckley et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=-120.0992+4.478 /(\mathrm{T} / \mathrm{K})+52.574 \cdot \log (\mathrm{~T} / \mathrm{K})-4.7697 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+1.5020 \times 10^{-5} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $489-873 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$0.0162 ; 7.64 \times 10^{-4}, 0.0617$ (liquid $\mathrm{P}_{\mathrm{L}}$ by GC-RT correlation; quoted $\mathrm{P}_{\mathrm{S}}$, converted to $\mathrm{P}_{\mathrm{L}}$, Donovan 1996)
0.0661 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$0.000144-0.00313 ; 0.000804-0.00511 ; 0.000683-0.00484$ (quoted exptl. values measured by: effusion, gas saturation; manometry, Delle Site 1997)
0.0049-0.00125; 0.000925-0.00129 (quoted lit. values by: calculation; from GC-RT relation, Delle Site 1997)
$8.69 \times 10^{-4 *}$ (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range $30-60^{\circ} \mathrm{C}$, Oja \& Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=33.281-12024 /(\mathrm{T} / \mathrm{K})$; temp range $318-363 \mathrm{~K}$ (Antoine eq., Knudsen effusion, Oja \& Suuberg 1998) $9.01 \times 10^{-2} ; 9.08 \times 10^{-4}$ (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.66-4380 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=8.39-2872 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid value, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{Pa})=12.977-4791.89 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
0.0724; 0.0442 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3780 /(\mathrm{T} / \mathrm{K})+11.54 ; \Delta \mathrm{H}_{\text {vap }}=-72.4 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
0.0014 (solid $\mathrm{P}_{\mathrm{S}}$, gas saturation-GC/MS, Mader \& Pankow 2003)
0.0922 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from $\mathrm{P}_{\mathrm{S}}$ assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Mader \& Pankow 2003)
$\ln (\mathrm{P} / \mathrm{Pa})=34.261-12339 /(\mathrm{T} / \mathrm{K})$; temp range 313-363 K (regression eq. of Hansen \& Eckert 1986 data, Li et al. 2004)
$\ln (\mathrm{P} / \mathrm{Pa})=(34.199 \pm 0.641)-(12332 \pm 229) /(\mathrm{T} / \mathrm{K})$; temp range $348-368 \mathrm{~K}$ (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
6.59 (gas stripping-GC, Southworth 1977, 1979)
7.19 (gas stripping-GC, Mackay \& Shiu 1981)
1.96 (wetted-wall column/GC, Fendinger \& Glotfelty 1990)
3.30 (gas stripping-GC, Friesen et al. 1993)
8.68 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
4.94* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Alaee et al. 1996)
$\ln \mathrm{K}_{\mathrm{AW}}=4.6774-3235.5 /(\mathrm{T} / \mathrm{K})$; temp range: $5.4-35.3^{\circ} \mathrm{C}$ (gas stripping-GC, Alaee et al. 1996)
5.64* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-5629.06 /(\mathrm{T} / \mathrm{K})+12.75, \Delta \mathrm{H}=46.8 \mathrm{~kJ} \mathrm{~mol}^{-1}$, measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=6.91-1363 /(\mathrm{T} / \mathrm{K})$, (Passivirta et al. 1999)
$4.58 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured data, Staudinger \& Roberts 2001)
$\log \mathrm{K}_{\mathrm{AW}}=2.065-1404 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
4.45 (Hansch \& Fujita 1964; Leo et al. 1971; Hansch \& Leo 1979)
4.67 (calculated-fragment const., Rekker 1977)
4.45 (calculated from Leo 1975, Southworth et al. 1978)
4.54 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
3.45 (HPLC-RT correlation, Veith 1979a)
4.34 (Kenaga \& Goring 1980)
4.49 (HPLC-k' correlation, McDuffie 1981)
4.38 (HPLC-k' correlation, Hanai et al. 1981)
4.63 (RP-TLC-k' correlation, Bruggeman et al. 1982)
4.20 (HPLC-k' correlation, D'Amboise 1982)
4.45 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
4.45 (RP-HPLC-RT correlation, Rapaport et al. 1984)
4.45 (shake flask-GC, Haky \& Leja 1986)
4.51 (HPLC-RT correlation, Eadsforth 1986)
4.63 (HPLC-RT correlation, Wang et al. 1986)
4.80 (HPLC-RT correlation, De Kock \& Lord 1987)
$4.50 \pm 0.15 \quad$ (recommended, Sangster 1989, 1993)
4.57 (TLC-RT correlation, De Voogt et al. 1990)
4.45 (recommended, Hansch et al. 1995)
$4.53 \pm 0.19,4.55 \pm 0.61 \quad$ (HPLC-k' correlation: ODS column, Diol column, Helweg et al. 1997)
4.68 (range 4.55-4.79) (shake flask-HPLC/fluo., De Maagd et al. 1998)
5.34 (RP-HPLC-RT correlation, short ODP column, Donovan \& Pescatore 2002)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ :
$7.30 \quad$ (calculated- $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, Wania \& Mackay 1996)
7.34 (calculated, Finizio et al. 1997)
7.55 (calculated- $\mathrm{S}_{\text {oct }}$ and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:

| $3.08,2.68$ | (Daphnia, pimephales, Southworth 1977) |
| :--- | :--- |
| 2.88 | (Daphnia pulex, Herbes \& Risi 1978) |
| 2.96 | (Daphnia pulex, Southworth et al. 1978) |
| 3.08 | (kinetic estimation, Southworth et al. 1978) |
| 3.89 | (algae, Geyer et al. 1981) |
| 4.22 | (P. hoyi, Eadie et al. 1982) |
| 3.67 | (microorganisms-water, Mabey et al. 1982) |
| 2.83 | (bluegill sunfish, Spacie et al. 1983) |
| 3.83 | (activated, sludge, Freitag et al. 1984) |
| 3.89 | (algae, Geyer et al. 1984) |
| 2.21 | (goldfish, Ogata et al. 1984) |
| $2.96,3.89,3.83$ | (fish, algae, activated sludge, Freitag et al. 1985) |
| 2.99 | (Daphnia magna, Newsted \& Giesy 1987) |
| $0.820,1.373$ | (Polychaete sp., Capitella capitata, Bayona et al. 1991) |

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
4.42 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
$3.74 \quad\left(22^{\circ} \mathrm{C}\right.$, suspended particulates, Herbes et al. 1980)
4.204 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
4.20 (soil, shake flask-UV, Karickhoff 1981)
3.95, 4.46 (Aldrich humic acid $9.4 \mathrm{mg} / \mathrm{L}$ DOC, RP-HPLC separation, equilibrium dialysis, Landrum et al. 1984)
3.95, 4.73 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with $9.6 \mathrm{mg} / \mathrm{L}$ DOC: Landrum et al. 1984)
4.87, 5.70 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Huron River with 7.8 $\mathrm{mg} / \mathrm{L}$ DOC, Landrum et al. 1984)
3.81, 4.87, 4.62, 4.20 (humic materials in natural water: Huron River $6.1 \%$ DOC spring, Huron river 6.7\% DOC winter, Grand River $10.7 \%$ DOC spring, Lake Michigan 5.5\% DOC spring, Lake Erie 9.6\% DOC spring, RP-HPLC separation method, Landrum et al. 1984)
4.20 (soil, shake flask-LSC, Nkedi-Kizza 1985)
4.93 (fluorescence quenching interaction with AB humic acid, Gauthier et al. 1986)
4.38 (HPLC-k' correlation, Hodson \& Williams 1988)
$4.21 \pm 0.11$ (Aldrich and Fluka humic acids, observed; Chin et al. 1989)
4.11 (soil-fine sand $0.2 \%$ OC, dynamic soil column studies, Enfield et al. 1989)
5.76 (sediments average, Kayal \& Connell 1990)
4.41 (RP-HPLC correlation, Pussemier et al. 1990)
4.53, 4.42 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
4.34, 4.38, 4.32 (RP-HPLC-k' correlation on different stationary phases, Szabo et al. 1995)
4.65 (humic acid, HPLC-k' correlation; Nielsen et al. 1997)
4.62 (4.60-4.64) (sediment from Lake Oostvaardersplassen, shake flask-HPLC/UV, de Maagd et al. 1998)
4.40; 4.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
4.36-5.97; 4.20-6.90 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$5.31 ; 5.33,5.12,4.92\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)
4.34; 4.26; 3.95-5.70 (calculated-K $\mathrm{K}_{\mathrm{ow}}$; calculated-solubility; quoted lit. range, Schlautman \& Morgan 1993a)
4.375 at $\mathrm{pH} 4,4.42$ at $\mathrm{pH} 7,4.39$ at pH 10 in $0.001 \mathrm{M} \mathrm{NaCl} ; 4.415$ at $\mathrm{pH} 4,4.37$ at $\mathrm{pH} 7,4.30$ at pH 10 in $0.01 \mathrm{M} \mathrm{NaCl} ; 4.50$ at $\mathrm{pH} 4,4.24$ at $\mathrm{pH} 7,4.27$ at pH 10 in $0.1 \mathrm{M} \mathrm{NaCl} ; 4.38$ at $\mathrm{pH} 4,4.40$ at $\mathrm{pH} 7,4.12$ at pH 10 in $1 \mathrm{mM} \mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautmam \& Morgan 1993a)
4.28 at $\mathrm{pH} 4,4.18$ at $\mathrm{pH} 7,4.24$ at pH 10 in $0.001 \mathrm{M} \mathrm{NaCl} ; 4.285$ at $\mathrm{pH} 4,4.15$ at $\mathrm{pH} 7,4.22$ at pH 10 in 0.01 $\mathrm{M} \mathrm{NaCl} ; 4.23$ at $\mathrm{pH} 4,4.12$ at $\mathrm{pH} 7,4.20$ at pH 10 in $0.1 \mathrm{M} \mathrm{NaCl} ; 4.21$ at $\mathrm{pH} 4,4.19$ at $\mathrm{pH} 7,4.24$ at pH 10 in $1 \mathrm{mM} \mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautmam \& Morgan 1993a)

## Environmental Fate Rate Constants, k , or Half-Lives, $\mathrm{t}_{1 / 2}$ :

Volatilization: removal rate constants from the water column at $25^{\circ} \mathrm{C}$ in midsummer sunlight were: $\mathrm{k}=0.002$ $\mathrm{h}^{-1}$ in deep, slow, somewhat turbid water; $\mathrm{k}=0.001 \mathrm{~h}^{-1}$ in deep, slow muddy water; $\mathrm{k}=0.002 \mathrm{~h}^{-1}$ in deep slow, clear water; $\mathrm{k}=0.042 \mathrm{~h}^{-1}$ in shallow, fast, clear water; and $\mathrm{k}=0.179 \mathrm{~h}^{-1}$ in very shallow, fast, clear water (Southworth 1977);
aquatic $\mathrm{t}_{1 / 2}=18-300 \mathrm{~h}$ (Callahan et al. 1979);
calculated $\mathrm{t}_{1 / 2}=62 \mathrm{~h}$ for a river 1-m deep with water velocity of $0.5 \mathrm{~m} / \mathrm{s}$ and wind velocity of $1 \mathrm{~m} / \mathrm{s}$ (Southworth 1979; quoted, Herbes et al. 1980; Hallett \& Brecher 1984).
Photolysis: removal rate constants from the water at $25^{\circ} \mathrm{C}$ in midsummer sunlight were: $\mathrm{k}=0.004 \mathrm{~h}^{-1}$ in deep, slow somewhat turbid water; $k<0.001 \mathrm{~h}^{-1}$ in deep, slow, muddy water; $\mathrm{k}=0.018 \mathrm{~h}^{-1}$ in deep, slow, clear water; $\mathrm{k}=0.086 \mathrm{~h}^{-1}$ in shallow, fast, clear water; and $\mathrm{k}=0.238 \mathrm{~h}^{-1}$ in very shallow, fast, clear water (Southworth 1977)
24-h photolytic $\mathrm{t}_{1 / 2} \sim 1.6 \mathrm{~h}$ in summer and $\mathrm{t}_{1 / 2}=4.8 \mathrm{~h}$ in winter at $35^{\circ} \mathrm{N}$ latitude (Southworth 1977)
direct sunlight $\mathrm{k}=0.15 \mathrm{~h}^{-1}$ in winter at $35^{\circ} \mathrm{N}$ latitude (Callahan et al. 1979)
$\mathrm{t}_{1 / 2}($ calc $)=0.75 \mathrm{~h}$ near surface water for direct sunlight photolysis at $40^{\circ} \mathrm{N}$ latitude of midday in midsummer (quoted, Herbes et al. 1980; Harris 1982)
$t_{1 / 2}=4.5 \mathrm{~d}$ in inland water, and $\mathrm{t}_{1 / 2}=5.2 \mathrm{~d}$ in inland water with sediment partitioning and $\mathrm{t}_{1 / 2}=0.75 \mathrm{~h}$ for direct photochemical transformation near water surface (Zepp \& Schlotzhauer 1979)
atmospheric and aqueous photolysis $t_{1 / 2}=0.58 \mathrm{~h}$, based on measured aqueous photolysis rate constant for midday summer sunlight at $35^{\circ} \mathrm{N}$ latitude (Southworth 1979; quoted, Howard et al. 1991) and adjusted for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
half-lives on different atmospheric particulate substrates (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=2.9 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=0.5 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=48 \mathrm{~h}$ on flyash (Behymer \& Hites 1985)
$t_{1 / 2}=4.5 \mathrm{~d}$ for summer at $40^{\circ} \mathrm{N}$ latitude under sunlight in surface water (Mill \& Mabey 1985)
$\mathrm{k}=0.66 \mathrm{~h}^{-1}$ in distilled water with $\mathrm{t}_{1 / 2}=1.0 \mathrm{~h}$ (Fukuda et al. 1988)
photodegradation $\mathrm{k}=0.023 \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=0.50 \mathrm{~h}$ for initial concentration of 5 ppm in methanol-water $(1: 1, \mathrm{v} / \mathrm{v})$ solution by high pressure mercury lamp or sunlight (Wang et al. 1991)
pseudo-first-order direct photolysis rate constants, $\mathrm{k}(\operatorname{exptl})=0.023 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=0.50 \mathrm{~h}$, and the predicted $\mathrm{k}=0.030 \mathrm{~min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
$\mathrm{k}=0.0503-0.0521 \mathrm{~min}^{-1}$ in natural water system by UV and sunlight (Yu et al. 1999)
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{calc})=3.10 \mathrm{~h}$, predicted by QSPR, in atmospheric aerosol (Chen et al. 2001)
Photodegradation $\mathrm{k}=4.7 \times 10^{-4} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant $k$, for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$
with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, $*$ data at other temperatures see reference:
photooxidation $t_{1 / 2}=1111-38500 \mathrm{~h}$, based on measured rate constant for reaction with hydroxyl radical in water (Radding et al. 1976; quoted, Howard et al. 1991)
k (aquatic) fate rate of $50 \mathrm{~L} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1600 \mathrm{~d}$ (Callahan et al. 1979)
k (calc) $=5.0 \times 10^{8} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet $\mathrm{O}_{2}$ and $2.2 \times 10^{5} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}(\mathrm{aq})=.3.3 \times 10^{-4} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=0.6 \mathrm{~h}$ under natural sunlight conditions (NRCC 1983)
$\mathrm{k}_{\mathrm{OH}}=110 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at $325 \pm 1 \mathrm{~K}$ (relative rate technique for propene, (Biermann et al. 1985; Atkinson 1989)
photooxidation $t_{1 / 2}=0.501-5.01 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987)
$\mathrm{k}_{\mathrm{OH}}($ calc $)=203 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ (molecular orbital calculations, Klamt 1996)
$\mathrm{k}=3.5 \times 10^{-5} \mathrm{~s}^{-1}$, indirect total photoreaction rate constant in surface waters (Mill 1999)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=190 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $306-366 \mathrm{~K}$ with a calculated atmospheric lifetime of 1.5 h based on gas-phase OH reaction (Brubaker \& Hites 1998)
Hydrolysis: $\mathrm{k}<0.001 \mathrm{~h}^{-1}$ at $25^{\circ} \mathrm{C}$ (Southworth 1977); not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation:
$\mathrm{k}=0.061 \mathrm{~h}^{-1}$ for microbial degradation in Third Creek water incubated 18 h at $25^{\circ} \mathrm{C}$; removal rate constants from water column at $25^{\circ} \mathrm{C}$ in midsummer sunlight were: $\mathrm{k}=0.060 \mathrm{~h}^{-1}$ in deep, slow, somewhat turbid water; $\mathrm{k}=0.030 \mathrm{~h}^{-1}$ in deep, slow, muddy water; $\mathrm{k}=0.061 \mathrm{~h}^{-1}$ in deep, slow, clear water; $\mathrm{k}=0.061 \mathrm{~h}^{-1}$ in shallow, fast, clear water; and $\mathrm{k}=0.061 \mathrm{~h}^{-1}$ in very shallow, fast, clear water (Southworth 1977)
$\mathrm{k}=0.035 \mathrm{~h}^{-1}$ for microbial degradation (Herbes et al. 1980; quoted, Hallett \& Brecher 1984)
significant degradation in 7 d with rapid adaptation for an average of three static-flask screening test (Tabak et al. 1981)
$\mathrm{k}=2.5 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=12 \mathrm{~d}$ and $\mathrm{k}=2.5 \times 10^{-4} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=115 \mathrm{~d}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (Herbes \& Schwall 1978, NRCC 1983)
$\mathrm{t}_{1 / 2}($ aq. aerobic $)=1200-11040 \mathrm{~h}$, based on aerobic soil die-away test data (Coover \& Sims 1987; Sims 1990; quoted, Howard et al. 1991)
$\mathrm{k}=0.0052 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=134 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0138 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=50 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
$\mathrm{t}_{1 / 2}($ aq. anaerobic $)=4800-44160 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation halflife (Howard et al. 1991).
Biotransformation: aquatic fate rate, $\mathrm{k}<0.0612 \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}>11.3 \mathrm{~h}$ (Callahan et al. 1979); estimated rate constant for bacteria of $3 \times 10^{-9} \mathrm{~mL}^{\text {cell }}{ }^{-1} \mathrm{~h}^{-1}$ (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\log \mathrm{k}_{1}=2.89 \mathrm{~h}^{-1} ; \log \mathrm{k}_{2}=0.0043 \mathrm{~h}^{-1}$ (Daphnia pulex, Herbes \& Risi 1978)
$\mathrm{k}_{1}=702 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.589 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)
$\mathrm{k}_{1}=\left(1.73 \times 10^{-3}-36\right) \mathrm{h}^{-1} ; \mathrm{k}_{2}=0.040 \mathrm{~h}^{-1}$ (average, bluegill sunfish, Spacie et al. 1983)
$\log \mathrm{k}_{1}=2.85 \mathrm{~h}^{-1}$; $\log \mathrm{k}_{2}=-0.23 \mathrm{~h}^{-1}$ (Daphnia pulex, correlated to Mackay \& Hughes 1984, Hawker \& Connell 1986)
$\mathrm{k}_{1}=1.46,16.9 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=(1.58-1.88) \times 10^{-3} \mathrm{~h}^{-1}$ (rainbow trout, Linder et al. 1985)
$\mathrm{k}_{1}=87.2 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.019 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, S. heringianus, Frank et al. 1986)
$\mathrm{k}_{1}=131.1 \mathrm{~mL} \mathrm{~g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0033 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, P. hoyi, Landrum 1988)
$\log \mathrm{k}_{2}=.2,-0.01 \mathrm{~d}^{-1}$ (fish, calculated $-\mathrm{K}_{\mathrm{ow}}$, Thomann 1989)
$\log \mathrm{k}_{2}=-0.96 \mathrm{~d}^{-1}$ (oyster, calculated- $\mathrm{K}_{\text {ow }}$, Thomann 1989)
$\mathrm{k}_{1}=1.8-2.3 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.045 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.58-1.7 \mathrm{~h}$, based on photolysis half-life in water (Howard et al. 1991);
half-lives under simulated atmospheric conditions: $\mathrm{t}_{1 / 2}=0.20 \mathrm{~h}$ for simulated sunlight, $\mathrm{t}_{1 / 2}=0.15 \mathrm{~h}$ for simulated sunlight + ozone with concn of $0.2 \mathrm{ppm}, \mathrm{t}_{1 / 2}=1.23 \mathrm{~h}$ for dark reaction ozone with concn of 0.2 ppm (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983);
calculated atmospheric lifetime of 1.5 h based on gas-phase OH reactions (Brubaker \& Hites 1998).
Surface water: half-lives for removal from water column at $25^{\circ} \mathrm{C}$ in midsummer sunlight were, $\mathrm{t}_{1 / 2}=10.5 \mathrm{~h}$ for
deep, slow, somewhat turbid water; $\mathrm{t}_{1 / 2}=21.6 \mathrm{~h}$ for deep, slow, muddy water; $\mathrm{t}_{1 / 2}=8.5 \mathrm{~h}$ for deep, slow, clear water; $t_{1 / 2}=3.5 \mathrm{~h}$ for shallow, fast, clear water; and $\mathrm{t}_{1 / 2}=1.4 \mathrm{~h}$ for very shallow, fast, clear water (Southworth 1977, Herbes et al. 1980);
computed near-surface $t_{1 / 2}=0.75 \mathrm{~h}$ of a water body and for direct photochemical transformation at latitude $40^{\circ} \mathrm{N}$, midday, midsummer and half-lives: $\mathrm{t}_{1 / 2}=4.5 \mathrm{~d}$ for no sediment-water partitioning, $\mathrm{t}_{1 / 2}=5.2 \mathrm{~d}$ with sediment-water partitioning and for direct photolysis in a $5-\mathrm{m}$ deep inland water body (Zepp \& Schlotzhauer 1979);
$\mathrm{t}_{1 / 2}=0.58-1.7 \mathrm{~h}$, based on photolysis half-life in water (Howard et al. 1991);
$\mathrm{t}_{1 / 2}=4.5 \mathrm{~d}$ at $40^{\circ} \mathrm{N}$ under summer sunlight (Mill \& Mabey 1985);
photolysis $\mathrm{t}_{1 / 2}=0.50 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);
indirect photoreaction $t_{1 / 2}=5.5 \mathrm{~h}$ in surface waters (Mill 1999);
photolysis $\mathrm{t}_{1 / 2}=13.3-13.80 \mathrm{~min}$ at $15^{\circ} \mathrm{C}$ in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater: $t_{1 / 2}=2400-22080 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: reduction $t_{1 / 2}=600 \mathrm{~h}$ for chemical available anthracene and $t_{1 / 2}=77 \mathrm{~h}$ for bioavailable anthracene for amphipod, $P$. hoyi in Lake Michigan sediments at $4^{\circ} \mathrm{C}$. The uptake clearance from sediment was $(0.024 \pm 0.002) \mathrm{g}$ of dry sediment $\cdot \mathrm{g}^{-1}$ of organism $\cdot \mathrm{h}^{-1}$, and the rate constants to become biologically unavailable were $(0.009 \pm 0.002) \mathrm{h}^{-1}$ corresponding to $\mathrm{t}_{1 / 2}=77 \mathrm{~h}$ (Landrum 1989).
Soil: $\mathrm{t}_{1 / 2}=3.3-175 \mathrm{~d}$ (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$t_{1 / 2}=17 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and $\mathrm{t}_{1 / 2}=45 \mathrm{~d}$ for $50 \mathrm{mg} / \mathrm{kg}$ treatment (Bulman et al. 1987);
degradation rate constant $\mathrm{k}=0.0052 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=134 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{k}=0.138 \mathrm{~d}^{-1}$ with $t_{1 / 2}=50 \mathrm{~d}$ for McLauren sandy loam soil (Park et al. 1990);
$\mathrm{t}_{1 / 2}=1200-11040 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991);
$\mathrm{t}_{1 / 2}=0.5-26 \mathrm{wk}, 7.9 \mathrm{yr}$ (quoted, Luddington soil, Wild et al. 1991).
Biota: $t_{1 / 2}=17 \mathrm{~h}$ in bluegill sunfish (Spacie et al. 1983);
with depuration $\mathrm{t}_{1 / 2}=37.75 \mathrm{~h}$ in $s$. heringianus (Frank et al. 1986);
elimination $\mathrm{t}_{1 / 2}=7 \mathrm{~d}$ from rainbow trout, $\mathrm{t}_{1 / 2}=1.9 \mathrm{~d}$ from mussel Mytilus edulis (quoted, Meador et al. 1995).

TABLE 4.1.1.25.1
Reported aqueous solubilities of anthracene at various temperatures and the reported empirical temperature dependence equations

$$
\begin{align*}
& \mathrm{R} \cdot \ln x=-\left[\Delta \mathrm{H}_{\mathrm{fu}} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{~T} / \mathrm{K})  \tag{1}\\
& \mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}  \tag{2}\\
& \ln x=\mathrm{A}-\mathrm{B} / \mathrm{T}(\mathrm{~K})  \tag{3}\\
& \ln x=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot \ln (\mathrm{~T} / \mathrm{K})  \tag{4}\\
& \ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau, \text { where } \tau=\mathrm{T} / \mathrm{T}_{\mathrm{o}}, \mathrm{~T}_{\mathrm{o}}=298.15 \mathrm{~K} \tag{4a}
\end{align*}
$$

1. 

| Wauchope \& Getzen 1972 |  |  |  | Schwarz 1977 |  | May et al. 1978a |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  |  |  | shake flask-fluorescence |  | generator column-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  | experimental |  | smoothed* |  |  |  |  |
| 35.4 | 0.125 | 0 | 0.022 | 8.60 | 0.0233 | 5.2 | 0.0127 |
| 35.4 | 0.122 | 25 | 0.075 | 11.1 | 0.0244 | 10.0 | 0.0175 |
| 35.4 | 0.119 | 35.4 | 0.123 | 12.2 | 0.0257 | 14.1 | 0.0222 |
| 39.3 | 0.152 | 39.3 | 0.159 | 14.0 | 0.0274 | 18.3 | 0.0291 |
| 39.3 | 0.151 | 44.7 | 0.214 | 15.5 | 0.0296 | 22.4 | 0.0372 |
| 39.3 | 0.148 | 47.5 | 0.249 | 19.2 | 0.0323 | 24.6 | 0.0434 |
| 44.7 | 0.208 | 50 | 0.286 | 20.3 | 0.0396 | 28.7 | 0.0557 |
| 44.7 | 0.210 | 50.1 | 0.288 | 23.3 | 0.0417 |  |  |
| 44.7 | 0.206 | 54.7 | 0.372 | 25.0 | 0.0410 |  |  |
| 47.5 | 0.279 | 59.2 | 0.481 | 26.2 | 0.0476 | temp dependence eq. 2 |  |
| 50.1 | 0.301 | 64.5 | 0.66 | 28.5 | 0.0579 | S | $\mu \mathrm{g} / \mathrm{kg}$ |
| 50.1 | 0.297 | 65.1 | 0.68 | 31.3 | 0.0695 | a | 0.0013 |
| 50.1 | 0.302 | 69.8 | 0.90 |  |  | b | -0.0097 |
| 54.7 | 0.391 | 70.7 | 0.95 |  |  | c | 0.8861 |
| 54.7 | 0.389 | 71.9 | 1.02 | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=34.81$ |  | d | 8.21 |
| 54.7 | 0.402 | 74.7 | 1.21 |  |  |  |  |
| 59.2 | 0.480 | 75.0 | 1.23 |  |  |  |  |
| 59.2 | 0.488 |  |  |  |  |  |  |
| 59.2 | 0.525 |  |  |  |  |  |  |
| 64.5 | 0.72 | mp dep | e eq. 1 |  |  |  |  |

TABLE 4.1.1.25.1 (Continued)

| Wauchope \& Getzen 1972 |  |  |  | Schwarz 1977 <br> shake flask-fluorescence |  | May et al. 1978a |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  |  |  |  |  | genera | mn-HPLC |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 64.5 | 0.62, 0.64 | $\ln x$ | mole fraction |  |  |  |  |
| 65.1 | 0.67, 0.64 | $\Delta \mathrm{H}_{\text {fus }}$ | $29.0 \pm 0.29$ |  |  |  |  |
| 69.8 | 0.92 | $10^{2} \cdot \mathrm{~b}$ | $1.81 \pm 0.15$ |  |  |  |  |
| 70.7 | 0.90, 0.97 | c | $19.3 \pm 0.5$ |  |  |  |  |
| 70.7 | 0.96 |  |  |  |  |  |  |
| 71.9 | 0.91 | $\Delta \mathrm{H}_{\text {fus }} /(\mathrm{kJ}$ | $)=29.0$ |  |  |  |  |
| 74.7 | 1.19, 1.13 |  |  |  |  |  |  |
| 74.7 | 1.26 |  |  |  |  |  |  |

2. 

| May et al. 1978b |  | May 1980 |  | May et al. 1983 |  | Velapoldi et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| generator column-HPLC |  | generator column-HPLC |  | generator column-HPLC |  | generator column-fluo. |  |
| $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 25 | 0.0446 | 5.2 | 0.0127 | 5.20 | 0.0127 | 10 | 0.0177 |
| 29 | 0.0579 | 10.0 | 0.0175 | 10.0 | 0.0175 | 15 | 0.02282 |
|  |  | 14.1 | 0.0222 | 14.1 | 0.0222 | 20 | 0.03061 |
| temp dependence eq. 2 |  | 18.3 | 0.0281 | 18.3 | 0.0291 | 25 | 0.04257 |
| S | $\mu \mathrm{g} / \mathrm{kg}$ | 22.4 | 0.0372 | 22.4 | 0.0372 | 30 | 0.06123 |
| a | 0.0013 | 24.6 | 0.0434 | 24.6 | 0.0434 |  |  |
| b | -0.0097 | 28.7 | 0.0557 | 28.7 | 0.0557 |  |  |
| c | 0.8861 |  |  | 9.70 | 0.0162 | eq. 4 | x |
| d | 8.21 |  |  | 16.6 | 0.0251 | A | -1078.056 |
|  |  | temp dependence eq. 2 |  | 23.2 | 0.0378 | B | 41884.5 |
| $\begin{aligned} & \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=43.76 \\ & \text { for temp range } 5-30^{\circ} \mathrm{C} \end{aligned}$ |  | S | $\mu \mathrm{g} / \mathrm{kg}$ | 29.3 | 0.0572 | C | 161.175 |
|  |  | a | 0.0013 |  |  |  |  |
|  |  | b | -0.0097 |  |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=51.3$ |  |
|  |  | c | 0.8886 |  |  |  |  |
|  |  | d | 8.21 |  |  |  |  |

3. 

| Whitehouse 1984 |  | Shaw 1989 |  | Reza et al. 2002 |  | Dohányosová et al. 2003 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| generator columnHPLC/UV |  | IUPAC recommended |  | generator columnHPLC/fluo |  | generator columnHPLC/UV |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{s} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 4.6 | 0.00961 | 0 | 0.022 | 8.94 | 0.0155 | 0.30 | 0.00963 |
| 8.8 | 0.0129 | 10 | 0.021 | 11.57 | 0.0183 | 5.0 | 0.0124 |
| 12.9 | 0.0177 | 20 | 0.034 | 13.39 | 0.0198 | 10 | 0.0169 |
| 17.0 | 0.0237 | 25 | 0.062* | 15.88 | 0.0246 | 15 | 0.0227 |
| 21.1 | 0.0323 | 30 | 0.080* | 22.54 | 0.0287 | 20 | 0.0320 |
| 25.3 | 0.0442 | 40 | 0.16* | 24.61 | 0.0434 | 25 | 0.0438 |
|  |  | 50 | 0.29* | 27.10 | 0.0505 | 30 | 0.0584 |
|  |  | 60 | 0.51* | 28.20 | 0.0540 | 35 | 0.0784 |
|  |  | 70 | 0.91* | 29.12 | 0.0565 | 40 | 0.106 |
|  |  |  |  | 30.53 | 0.0633 | 45 | 0.145 |

(Continued)



FIGURE 4.1.1.25.1 Logarithm of mole fraction solubility $(\ln x)$ versus reciprocal temperature for anthracene.

TABLE 4.1.1.25.2
Reported vapor pressures of anthracene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
1.

2.

| Bradley \& Cleasby 1953 |  | Kelley \& Rice 1964 |  | Malaspina et al. 1973 |  | Power et al. 1977 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| effusion |  | effusion |  | Knudsen effusion |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 65.7 | 0.115 | data represented by |  | 79.55 | 0.612 | 30 | 0.00937 |
| 69.91 | 0.167 |  |  | 88.25 | 1.373 | 30 | 0.00913 |
| 73.35 | 0.259 | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | 98.05 | 3.506 | 50 | 0.0928 |


| TABLE 4.1.1.25.2 (Continued) |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Bradley \& Cleasby 1953 |  | Kelley \& Rice 1964 |  | Malaspina et al. 1973 |  | Power et al. 1977 |  |
| effusion |  | effusion |  | Knudsen effusion |  | gas saturation |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathbf{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 79.95 | 0.489 | A | 12.068 | 105.95 | 6.413 | 70 | 0.582 |
| 67.1 | 0.140 | B | 5145 | 113.75 | 12.17 | 70 | 0.5826 |
| 68.75 | 0.157 | measur | $69-86^{\circ} \mathrm{C}$ | 123.75 | 29.33 | 100 | 7.738 |
| 71.25 | 0.208 | $\Delta \mathrm{H}_{\text {fus }} /$ | $=93.91$ | 135.25 | 61.06 | 100 | 7.771 |
| 73.2 | 0.223 |  |  | 142.35 | 106.32 |  |  |
| 80.4 | 0.524 | reported | ated data | 149.75 | 189.31 |  |  |
|  |  | 95 | 1.667 | 159.15 | 483.95 | eq. 2 | $\mathrm{P} / \mathrm{mmHg}$ |
|  |  | 100 | 2.546 |  |  | A | 36.40 |
| eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | 105 | 3.880 |  |  | B | 8634 |
| A | 11.638 |  |  | eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ | C | 238.6 |
| B | 5320 |  |  | A | 12.616 |  |  |
|  |  |  |  | B | 5277 |  |  |

3. 

| Macknick \& Prausnitz 1979 |  |  | 1980 | Grayson | raey 1982 | Sonnefeld et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation-GC |  | teorsion-, | ing effusion | gas saturation-GC |  | gas saturation-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |
| 85.25 | 0.892 | 64.44 | 0.10 | 20.0 | 0.00102 | 12.3 | $1.64 \times 10^{-4}$ |
| 90.15 | 1.36 | 71.18 | 0.20 | 50.1 | 0.035 | 12.3 | $1.57 \times 10^{-4}$ |
| 95.65 | 2.13 | 75.20 | 0.30 | 60.0 | 0.0849 | 12.3 | $1.60 \times 10^{-4}$ |
| 100.7 | 3.32 | 78.12 | 0.40 | 70.0 | 0.267 | 19.2 | $3.76 \times 10^{-4}$ |
| 104.7 | 4.59 | 80.41 | 0.50 | 75.0 | 0.359 | 19.2 | $3.83 \times 10^{-4}$ |
| 111.9 | 8.04 | 82.31 | 0.60 | 80.5 | 0.588 | 19.2 | $3.54 \times 10^{-4}$ |
| 116.4 | 11.41 | 83.93 | 0.70 |  |  | 19.2 | $3.72 \times 10^{-4}$ |
| 119.93 | 14.67 | 85.35 | 0.80 |  |  | 25.0 | $8.43 \times 10^{-4}$ |
|  |  | 86.61 | 0.90 | eq. 1 | $\mathrm{P} / \mathrm{Pa}$ | 25.0 | $8.17 \times 10^{-4}$ |
|  |  | 87.74 | 1.00 | A | 30.5 | 25.0 | $8.19 \times 10^{-4}$ |
| eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |  |  | B | 10968 | 25.0 | $3.30 \times 10^{-4}$ |
| A | 26.805 | 25.0 | 0.00875 |  |  | 30.1 | $1.46 \times 10^{-3}$ |
| B | 111402 |  | extrapolated |  |  | 30.1 | $1.54 \times 10^{-3}$ |
|  |  |  |  |  |  | 30.1 | $1.51 \times 10^{-3}$ |
|  |  | $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{k}$ | $\left.{ }^{-1}\right)=100.4$ |  |  | 34.93 | $2.59 \times 10^{-3}$ |
|  |  |  |  |  |  | 34.93 | $2.63 \times 10^{-3}$ |
|  |  |  |  |  |  | 34.93 | $2.69 \times 10^{-3}$ |
|  |  |  |  |  |  | eq. 1 | $\mathrm{P} / \mathrm{Pa}$ |
|  |  |  |  |  |  | A | 12.977 |
|  |  |  |  |  |  | B | 4891.87 |

TABLE 4.1.1.25.2 (Continued)
4.

| Bender et al. 1983 |  | Rordorf 1985 |  | Hansen \& Eckert 1986 |  | Oja \& Suuberg 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| gas saturation |  | gas saturation-GC |  | gas saturation-IR |  | Knudsen effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $t /{ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 80.45 | 0.55 | 25 | 0.00106 | 40 | 0.0058 | 27.7 | 0.00114 |
| 82.05 | 0.67 | 50 | 0.023 | 45 | 0.0105 | 39.7 | 0.00575 |
| 85.35 | 0.864 | 75 | 0.322 | 50 | 0.0193 | 47.6 | 0.0162 |
| 90.5 | 1.418 | 100 | 3.17 | 55 | 0.039 | 54.6 | 0.0355 |
| 94.5 | 2.019 | 125 | 23.4 | 60 | 0.0675 | 60.1 | 0.062 |
| 100.8 | 3.426 | 150 | 136.2 | 65 | 0.0987 | 72.7 | 0.204 |
| 105.65 | 4.99 |  |  | 70 | 0.1688 | 74.1 | 0.258 |
| 110.4 | 7.17 | $\Delta \mathrm{H}_{\text {subl }} /$ | $\left.{ }^{-1}\right)=98.75$ | 75 | 0.3056 |  |  |
| 115.35 | 10.01 |  |  | 80 | 0.5252 | eq. 1a | P/Pa |
| 115.65 | 10.58 | av. selec | ature value | 85 | 0.9247 | A | 33.281 |
| 110.857 | 15.30 | 25 | 0.00108 | 90 | 1.244 | B | 12024 |
| 125.45 | 21.30 | 50 | 0.0243 |  |  |  |  |
|  |  | 75 | 0.344 |  |  | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=100.0$ |  |
| eq. 1 | $\mathrm{P} / \mathrm{Pa}$ | 100 | 3.38 | eq. 1 | $\mathrm{P} / \mathrm{mPa}$ |  |  |
| A | 31.620 | 125 | 24.5 | A | 17.88 |  |  |
| B | 1138 | 150 | 139.7 | B | 5359 |  |  |
|  |  | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=98.79$ |  | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=102.6$ |  |  |  |



FIGURE 4.1.1.25.2 Logarithm of vapor pressure versus reciprocal temperature for anthracene.

## TABLE 4.1.1.25.3

Reported Henry's law constants of anthracene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$

$$
\begin{align*}
& \log K_{A W}=A-B /(T / K)  \tag{1}\\
& \log \left(1 / K_{A W}\right)=A-B /(T / K) \tag{2}
\end{align*}
$$

$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

| Alaee et al. 1996 |  | Bamford et al. 1999 |  |  |
| :---: | :---: | :---: | :---: | :---: |
| gas stripping-GC |  | gas stripping-GC/MS |  |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m³/mol) | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) |
|  |  |  |  | average |
| 5.4 | 2.76 | 4.1 | 1.14, 1.38 | 1.25 |
| 10.1 | 3.12 | 11.0 | 1.99, 2.26 | 2.12 |
| 14.8 | 3.44 | 18.0 | 3.31, 3.70 | 3.50 |
| 20.6 | 3.91 | 25.0 | 5.26, 6.06 | 5.64 |
| 25.0 | 4.94 | 31.0 | 7.60, 9.18 | 8.36 |
| 30.2 | 8.05 |  |  |  |
| 34.3 | 8.94 | eq. 1 | $\mathrm{K}_{\text {AW }}$ |  |
|  |  | A | 12.75 |  |
| eq. 1 | $\mathrm{K}_{\mathrm{AW}}$ | B | 5629 |  |
| A | $4.680$ |  |  |  |
| B | $3235.5$ |  | ropy change: |  |
|  |  |  | $=46.8 \pm 1.7$ |  |
| enthalpy of volatilization: |  |  | $\left.\mathrm{ol}^{-1}\right)=106$ |  |
| $\Delta \mathrm{H}_{\mathrm{vol}} /\left(\mathrm{kJ} \cdot \mathrm{~mol}^{-1}\right)=26.9$ |  |  | at $25^{\circ} \mathrm{C}$ |  |



FIGURE 4.1.1.25.3 Logarithm of Henry's law constant versus reciprocal temperature for anthracene.

### 4.1.1.26 2-Methylanthracene



Common Name: 2-Methylanthracene Synonym:
Chemical Name: 2-methylanthracene
CAS Registry No: 613-12-7
Molecular Formula: $\mathrm{C}_{15} \mathrm{H}_{12}$
Molecular Weight: 192.256
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
209 (Weast 1982-83; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
359 (sublimation, Bjørseth 1983)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
$1.80 \quad\left(0^{\circ} \mathrm{C}\right.$, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
106 (calculated-density, liquid molar volume, Lande \& Banerjee 1981) 218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0157 ( mp at $209^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.039 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.0219* (generator column-HPLC/UV, measured range $6.3-31.1^{\circ} \mathrm{C}$, May et al. 1978a)
0.0213 (generator column-HPLC/UV, measured range $5-30^{\circ} \mathrm{C}$, May et al. 1978b)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=324.0+5.413 \cdot\left(\mathrm{t} /{ }^{\circ}\right)+0.8059 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0025 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $5-30^{\circ} \mathrm{C}$ (generator columnHPLC/UC, May et al. 1978b)
$0.0191^{*} \quad\left(23.1^{\circ} \mathrm{C}\right.$, generator column-HPLC/fluo., temp range $278.25-302.45 \mathrm{~K}$, May et al. 1983)
0.031 (average lit. value, Pearlman et al. 1984)
$0.0225^{*} \quad$ (generator column-HPLC/UV, measured range $4.6-25.3^{\circ} \mathrm{C}$, Whitehouse 1984)
0.03* (tentative value, IUPAC Solubility Data Series, Shaw 1989)
$\ln x=-1.841995-4616.86 /(\mathrm{T} / \mathrm{K})$, temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
0.0262* (generator column-HPLC/UV, measured range $0-50^{\circ} \mathrm{C}$, Dohányosová et al. 2003)
$\ln x=-42.7975+22.9752 / \tau+\mathrm{C} \ln \tau, \tau=\mathrm{T} / 298.15 \mathrm{~K}$; temp range $0-50^{\circ} \mathrm{C}$ (generator column-HPLC/UV,
Dohányosová et al. 2003)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
0.0207 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3976 /(\mathrm{T} / \mathrm{K})+11.65 ; \Delta \mathrm{H}_{\text {vap. }}=-76.1 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations:
5.15 (calculated-fragment const., Yalkowsky \& Valvani 1979,1980)
5.00 (shake flask-UV, Alcorn et al. 1993)
5.00 (recommended, Sangster 1993)
4.97; 4.70 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)
$\log \mathrm{K}_{\mathrm{ow}}=1.093+1154.2 /(\mathrm{T} / \mathrm{K})$; temp range $5-55^{\circ} \mathrm{C}$ (temperature dependence HPLC- $\mathrm{k}^{\prime}$ correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, $k$ or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Hydrolysis:
Oxidation:
Half-Lives in the Environment:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from rainbow trout (quoted, Meador et al. 1995).

## TABLE 4.1.1.26.1

Reported aqueous solubilities of 2-methylanthracene at various temperature and the empirical temperature dependence equations

| $\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}$ | (1) |
| :--- | :--- |
| $\ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau$ | (2) $\quad$ where $\tau=\mathrm{T} / \mathrm{T}_{\mathrm{o}}$ and $\mathrm{T}_{\mathrm{o}}=298.15 \mathrm{~K}$ |


| May et al. 1978a, May 1983 |  | Whitehouse 1984 |  | Shaw 1989b |  | Dohányosová et al. 2003 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| generator column-HPLC |  | generator column-HPLC/UV |  | IUPAC "tentative" values |  | generator column-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 6.3 | 0.00706 | 4.6 | - | 5 | 0.006 | 0.30 | 0.00567 |
| 9.1 | 0.00848 | 8.8 | 0.00754 | 10 | 0.009 | 5.0 | 0.00738 |
| 10.8 | 0.00943 | 12.9 | 0.00969 | 20 | 0.016 | 20 | 0.0106 |
| 13.9 | 0.0111 | 17.0 | 0.0123 | 25 | 0.03 | 15 | 0.0142 |
| 18.3 | 0.0145 | 21.1 | 0.0161 | 30 | 0.03 | 20 | 0.0192 |
| 23.1 | 0.0191 | 25.3 | 0.0225 |  |  | 25 | 0.0262 |
| 27.0 | 0.0242 |  |  |  |  | 30 | 0.0352 |
| 31.1 | 0.0321 |  |  |  |  | 35 | 0.048 |
|  |  |  |  |  |  | 40 | 0.0674 |
| temp | eq. 1 |  |  |  |  | 45 | 0.0943 |
| S | $\mu \mathrm{g} / \mathrm{kg}$ |  |  |  |  | 50 | 0.125 |
| a | 0.0011 |  |  |  |  |  |  |
| b | -0.0306 |  |  |  |  | eq. 2 | x |
| c | 0.8180 |  |  |  |  | A | -42.7975 |
| d | 2.78 |  |  |  |  | B | 22.9752 |
| $\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=39.08$ <br> measured between $5-30^{\circ} \mathrm{C}$ |  |  |  |  |  | C | 41.7206 |
|  |  |  |  |  |  | $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=46.15 \pm 0.3 \\ & 0.3 \end{aligned}$ |  |
|  |  |  |  |  |  |  | at 298.15 K |
|  |  |  |  |  |  | $\mathrm{mp} / \mathrm{K}$ | 479 |
|  |  |  |  |  |  | $\Delta \mathrm{H}_{\text {fus }} /(\mathrm{kJ} \mathrm{m}$ | $=24.06$ |



FIGURE 4.1.1.26.1 Logarithm of mole fraction solubility ( $\ln \mathrm{x}$ ) versus reciprocal temperature for 2-methylanthracene.

### 4.1.1.27 9-Methylanthracene



Common Name: 9-Methylanthracene
Synonym:
Chemical Name: 9-methylanthracene
CAS Registry No: 779-02-2
Molecular Formula: $\mathrm{C}_{15} \mathrm{H}_{12}$
Molecular Weight: 192.256
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
81.5 (Weast 1982-83; Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
$196(12 \mathrm{~mm} \mathrm{Hg}$, Weast 1982-83; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.065 \quad\left(99^{\circ} \mathrm{C}\right.$, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
181 (calculated-density, liquid molar volume, Lande \& Banerjee 1981) 218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.279\left(\mathrm{mp}\right.$ at $81.5^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.261 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.269 (average lit. value, Pearlman et al. 1984)
0.530 (generator column-HPLC, Vadas et al. 1991)
$0.0376^{*}$ (generator column-HPLC/UV, measured range $0-50^{\circ} \mathrm{C}$, Dohányosová et al. 2003)
$\ln x=-76.9798+59.8386 / \tau+\mathrm{C} \ln \tau, \tau=\mathrm{T} / 298.15 \mathrm{~K}$, temp range $0-50^{\circ} \mathrm{C}$ (generator column-HPLC/UV,
Dohányosová et al. 2003)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
0.00224 (extrapolated-Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=11.683-5168 /(\mathrm{T} / \mathrm{K})$; temp range $354-402 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
5.12 (calculated $-\pi$ const., Southworth et al. 1978)
5.07 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
5.15 (calculated-fragment const., Valvani \& Yalkowsky 1980; Yalkowsky \& Valvani 1979,1980)
5.14 (average lit. value, Yalkowsky et al. 1983)
5.61 (HPLC-RT correlation; Burkhard et al. 1985)
5.10 (HPLC-RT correlation, Wang et al. 1986)
$5.07 \pm 0.20$ (recommended, Sangster 1989, 1993)
5.07 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
3.66; 3.59 (Daphnia pulex; kinetic estimation, Southworth et al. 1978)
(calculated-K ${ }_{\text {Ow }}$, Mackay 1982)
(calculated-MCI $\chi$, calculated- $\mathrm{K}_{\mathrm{OW}}$, Lu et al. 1999)
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}:$
4.81 (natural sediment, average of isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
4.50 (calculated-molecular connectivity indices $\chi$, Sabljic 1984)
4.81 (calculated-MCI ${ }^{1} \chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
$t_{1 / 2}($ calc $)=0.13 \mathrm{~h}$ for direct photochemical transformation near water surface and $t_{1 / 2}=0.78 \mathrm{~d}$ for no sedimentwater partitioning; and $t_{1 / 2}=1.2 \mathrm{~d}$ with sediment-water partitioning (Zepp \& Scholtzhauer 1979)
$\mathrm{t}_{1 / 2}=0.79 \mathrm{~d}$ for summer at $40^{\circ} \mathrm{N}$ latitude under sunlight in surface water (Mill \& Mabey 1985)
photodegradation $\mathrm{k}=0.163 \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=0.07 \mathrm{~h}$ in methanol-water ( $2: 3, \mathrm{v} / \mathrm{v}$ ) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
the pseudo-first-order direct photolysis $\mathrm{k}(\operatorname{exptl})=0.0163 \mathrm{~min}^{-1}$ with calculated $\mathrm{t}_{1 / 2}=0.07 \mathrm{~h}$ and the predicted $\mathrm{k}($ calc $)=0.00343 \mathrm{~min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
direct photolysis $\mathrm{t}_{1 / 2}=1.85 \mathrm{~h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
Oxidation: $t_{1 / 2}=10 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
$\mathrm{k}_{1}=561 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.144 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)
$\log \mathrm{k}_{1}=2.75 \mathrm{~h}^{-1} ; \log \mathrm{k}_{2}=-0.84 \mathrm{~h}^{-1}$ (Daphnia pulex, correlated as per Mackay \& Highes 1984, Hawker \& Connell 1986)

Half-Lives in the Environment:
Air: direct photolysis $\mathrm{t}_{1 / 2}=1.85 \mathrm{~h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
Surface water: computed $t_{1 / 2}=0.13 \mathrm{~h}$ at near-surface of a water body, for direct photochemical transformation, and $t_{1 / 2}=0.79 \mathrm{~d}$ for direct photolysis in a $5-\mathrm{m}$ deep inland water body with no sediment-water partitioning, $\mathrm{t}_{1 / 2}=1.2 \mathrm{~d}$ with sediment-water partitioning to top cm bottom sediment; and $\mathrm{t}_{1 / 2}=10 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979);
$\mathrm{t}_{1 / 2}=0.79 \mathrm{~d}$ for summer at $40^{\circ} \mathrm{N}$ latitude under sunlight (Mill \& Mabey 1985);
photolysis $t_{1 / 2}=0.07 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1 / 2}=4 \mathrm{~d}$ from rainbow trout (quoted, Meador et al. 1995).

## TABLE 4.1.1.27.1

Reported aqueous solubilities of 9-methylanthracene at various temperature and the empirical temperature dependence equations

$$
\begin{equation*}
\ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau \text {, where } \tau=\mathrm{T} / \mathrm{T}_{\mathrm{o}} \text { and } \mathrm{T}_{\mathrm{o}}=298.15 \mathrm{~K} \tag{1}
\end{equation*}
$$

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| Generator column-HPLC |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 0.30 | 0.113 |
| 5.0 | 0.137 |
| 20 | 0.174 |
| 15 | 0.228 |
| 20 | 0.286 |
| 25 | 0.376 |
| 30 | 0.508 |
| 35 | 0.699 |
| 40 | 0.953 |
| 45 | 1.270 |
| 50 | 1.770 |
| $\mathrm{eq} 1$. | mole fraction |
| A | -76.9798 |
| B | 59.8386 |
| C | 76.7066 |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=41.8 \pm 0.2$ |  |
| $\mathrm{mp} / \mathrm{K}$ | at 298.15 K |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=16.95$ |  |



FIGURE 4.1.1.27.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 9methylanthracene.

### 4.1.1.28 9,10-Dimethylanthracene



Common Name: 9,10-Dimethylanthracene Synonym:
Chemical Name: 9,10-dimethylanthracene
CAS Registry No: 781-43-1
Molecular Formula: $\mathrm{C}_{16} \mathrm{H}_{14}$
Molecular Weight: 206.282
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
183.6 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
360 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
241.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0278 (at $\mathrm{mp}=183.6^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.056 (shake flask-fluorescence, Mackay \& Shiu 1977)
$0.0129^{*}$ (generator column-HPLC/UV, measured range $0-50^{\circ} \mathrm{C}$, Dohányosová et al. 2003)
$\ln x=-73.2594+52.6685 / \tau+\mathrm{C} \ln \tau, \tau=\mathrm{T} / 298.15 \mathrm{~K}$; temp range $0-50^{\circ} \mathrm{C}$ (generator column-HPLC/UV,
Dohányosová et al. 2003)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$1.53 \times 10^{-4}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.266-5391 /(\mathrm{T} / \mathrm{K})$; temp range 381-434 K (Antoine eq., Stephenson \& Malanowski 1987)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
5.69 (HPLC-RT correlation, Wang et al. 1986)
5.69 (recommended, Sangster 1989, 1993)
5.69 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: direct photochemical transformation $\mathrm{t}_{1 / 2}($ calc $)=0.35 \mathrm{~h}$, computed near-surface water, latitude $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
photodegradation in methanol-water ( $2: 3, \mathrm{v} / \mathrm{v}$ ) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight with a rate constant $\mathrm{k}=0.0633 \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=0.18 \mathrm{~h}$ (Wang et al. 1991)
pseudo-first-order direct photolysis $\mathrm{k}(\operatorname{exptl})=0.0633 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=0.18 \mathrm{~h}$ and the predicted $\mathrm{k}($ calc $)=0.0379 \mathrm{~min}^{-1}$ calculated by QSPR metnod in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
direct photolysis $t_{1 / 2}=1.17 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).
Oxidation: $t_{1 / 2}=1.5 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
Half-Lives in the Environment:
Air: direct photolysis $t_{1 / 2}=1.17 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).
Surface water: photolysis $\mathrm{t}_{1 / 2}=0.35 \mathrm{~h}$ near surface water, $40^{\circ} \mathrm{N}$; midday, midsummer and photosensitized oxygenation $t_{1 / 2}=1.5 \mathrm{~h}$ at near surface water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979).
photolysis $t_{1 / 2}=0.18 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp
(Chen et al. 1996).
Groundwater:
Sediment:
Soil:
Biota:

TABLE 4.1.1.28.1
Reported aqueous solubilities of 9,10-dimethylanthracene at various temperature and the empirical temperature dependence equations

$$
\begin{equation*}
\ln x=\mathrm{A}+\mathrm{B} / \tau+\mathrm{C} \ln \tau \text {, where } \tau=\mathrm{T} / \mathrm{T}_{\mathrm{o}} \text { and } \mathrm{T}_{\mathrm{o}}=298.15 \mathrm{~K} \tag{1}
\end{equation*}
$$

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| generator column- $\mathbf{H P L C}$ |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 0.30 | 0.000391 |
| 5.0 | 0.00382 |
| 20 | 0.00534 |
| 15 | 0.00698 |
| 20 | 0.00932 |
| 25 | 0.0129 |
| 30 | 0.0186 |
| 35 | 0.0252 |
| 40 | 0.0351 |
| 45 | 0.0501 |
| 50 | 0.0728 |
| eq .1 | mole fraction |
| A | -73.2594 |
| B | 52.6685 |
| C | 71.9873 |
|  |  |
| $\Delta \mathrm{H}_{\text {sol }} /(\mathrm{kJ} \mathrm{mol}$ |  |
|  |  |
| $\mathrm{mp} / \mathrm{K}$ | $47.9 \pm 0.3$ |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=23.46$ | at 298.15 K |



FIGURE 4.1.1.28.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for 9, 10-dimethylanthracene.

### 4.1.1.29 Pyrene



Common Name: Pyrene
Synonym: benzo[def]phenanthrene
Chemical Name: pyrene
CAS Registry No: 129-00-0
Molecular Formula: $\mathrm{C}_{16} \mathrm{H}_{10}$
Molecular Weight: 202.250
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
150.62 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 404 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.271 \quad\left(23^{\circ} \mathrm{C}\right.$, Weast 1982-83; Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
159.0 (calculated-density, liquid molar volume, Lande \& Banerjee 1981)
213.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
17.11 (Ruelle \& Kesselring 1997)
$0.29,17.36 ; 17.65 \quad\left(-152.35,150.65^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
35.98 (Wauchope \& Getzen 1972)
40.17 (Casellato et al. 1973)
54.8 (Hinckley et al. 1990)
$40.97 \quad\left(150.65^{\circ} \mathrm{C}\right.$, Chickos et al. 1999)
43.36, 43.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0585\left(\mathrm{mp}\right.$ at $150.62^{\circ} \mathrm{C}$ )
0.128 (calculated, $\Delta \mathrm{S}_{\text {fus }}=40.3 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.165 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.175 (shake flask-UV, Klevens 1950)
0.148 (Pierotti et al. 1959)
1.56 (shake flask-UV/fluorescence, Barone et al. 1967)
$0.105 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
0.148* (shake flask-UV, measured range $22.2-74.7^{\circ} \mathrm{C}$, Wauchope \& Getzen 1972)
$\mathrm{R} \cdot \ln x=-3660 /(\mathrm{T} / \mathrm{K})+4.08 \times 10^{-4} \cdot[(\mathrm{~T} / \mathrm{K})-291.15]^{2}-38.1+0.0478 \cdot(\mathrm{~T} / \mathrm{K})$; temp range $22.2-73.4^{\circ} \mathrm{C}$ (shake flask-UV measurements, Wauchope \& Getzen 1972)
$0.105,0.133,0.107,0.069$ (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)
0.171 (shake flask-fluorescence/UV, Schwarz \& Wasik 1976)
0.135 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.132 (Rossi 1977; Neff 1979)
$0.1295^{*} \quad$ (shake flask-fluorescence, measured range $12.2-31.3^{\circ} \mathrm{C}$, Schwarz 1977)
0.132* (generator column-HPLC/UV, measured range $5-30^{\circ} \mathrm{C}$, May et al. 1978b)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=50.2-1.051 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+0.2007 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}-0.0011 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $5-30^{\circ} \mathrm{C}$ (generator columnHPLC/UV, May et al. 1978b)
0.032 (shake flask-nephelometry, Hollifield 1979)
0.135 (shake flask-LSC, Means et al. 1979; 1980)
0.130 (shake flask-GC/UV, Rossi \& Thomas 1981)
0.136* $\quad\left(25.5^{\circ} \mathrm{C}\right.$, generator column-HPLC/UV, measured range 277.85-303.05 K, May et al. 1983)
0.129 (average lit. value, Pearlman et al. 1984)
0.133 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
0.135 (RP-HPLC-RT correlation, Chin et al. 1986)
0.118 (generator column-HPLC/UV, Billington et al. 1988)
0.132* (recommended, IUPAC Solubility Data Series, Shaw 1989)
0.150 (shake flask-LSC, Eadie et al. 1990)
0.107 (generator column-HPLC, Vadas et al. 1991)
$0.132,0.050\left(\right.$ solid $\mathrm{S}_{\mathrm{S}}$ at $26^{\circ} \mathrm{C}$ ); 2.61, 1.01 (supercooled liquid $\mathrm{S}_{\mathrm{L}}$ at $4^{\circ} \mathrm{C}$ ) (quoted, Piatt et al. 1996)
0.131 ; $0.077,0.422$ (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)
0.150 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=0.316-895.4 /(\mathrm{T} / \mathrm{K})$; (supercooled liquid, Passivirta et al. 1999)
$\ln x=-4.007476-4252.03 /(\mathrm{T} / \mathrm{K})$, temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
$0.1331^{*} \quad\left(25.55^{\circ} \mathrm{C}\right.$, generator column-HPLC/fluorescence, measured range $0.75-32.08^{\circ} \mathrm{C}$, Reza et al. 2002)
$\ln x=(-1.30 \pm 0.56)+(-5059 \pm 165) /(\mathrm{T} / \mathrm{K})$; temp range $281.9-305.23 \mathrm{~K}$ (Reza et al. 2002)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$\begin{array}{ll}0.00339 & \text { (effusion method, Inokuchi et al. 1952) } \\ 0.000882^{*} & \text { (effusion method, extrapolated from Antoine eq., Bradley \& Cleasby 1953) }\end{array}$
$\log (\mathrm{P} / \mathrm{cmHg})=10.270-4904 /(\mathrm{T} / \mathrm{K})$; temp range $71.75-85.25^{\circ} \mathrm{C}$ (Antoine eq., Bradley \& Cleasby 1953)
347* $\quad\left(200.4^{\circ} \mathrm{C}\right.$, temp range $200.4-394.7^{\circ} \mathrm{C}$, Tsypkina 1955 ; quoted, Boublik et al. 1984)
0.00033 (effusion method, Hoyer \& Peperle 1958; quoted, Mabey et al. 1982; Tsai et al. 1991)
$\log (\mathrm{P} / \mathrm{mmHg})=12.0-5248 /(\mathrm{T} / \mathrm{K})$, temp range $25-90^{\circ} \mathrm{C}$, (Knudsen effusion method, Hoyer \& Peperle 1958)
0.2118* (348 K, Knudsen effusion, measured range 348-419 K, Malaspina et al. 1974)
12.4* $\quad\left(125^{\circ} \mathrm{C}\right.$, inclined-piston gauge, measured range $125-185^{\circ} \mathrm{C}$, Smith et al. 1980)
0.00091 (effusion method, Pupp et al. 1974; quoted, Bidleman 1984)
0.00027 (lit. average-interpolated, API 1979; quoted, Wasik et al. 1983)
0.00088 (extrapolated from Antoine eq., Amidon \& Anik 1981)
0.00060* (gas saturation-HPLC/fluo./UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=12.748-4760.73 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (solid, Antoine eq., Sonnefeld et al. 1983)
0.0006 (generator column-HPLC/fluo./UV, Wasik et al. 1983)
$0.0113,0.0049 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
0.0158 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with $\Delta \mathrm{S}_{\text {fus }}$ Bidleman 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=4.75092-1127.529 /\left(16.02+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $200-394^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$0.00442 \quad$ (Yamasaki et al. 1984)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=5.6184-1122.0 /\left(15.2+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $200-395^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985 , 1992)
0.00033 (selected, Howard et al. 1986; quoted, Banerjee et al. 1990)
0.00055 (interpolated Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.75452-5072.78 /(\mathrm{T} / \mathrm{K})$; temp range $298-401 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.35032-5286.784 /(\mathrm{T} / \mathrm{K})$; temp range $360-419 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=5.5106-1743.57 /(-170.83+\mathrm{T} / \mathrm{K})$, temp range $513-668 \mathrm{~K}$, (Antoine eq.-III, Stephenson \& Malanowski 1987)
$0.000413,0.00973$ (lit. mean, supercooled liquid value $\mathrm{P}_{\mathrm{L}}$, Bidleman \& Foreman 1987)
0.000293* (pressure gauge, extrapolated-Antoine eq. derived exptl. data, temp 80-140 ${ }^{\circ} \mathrm{C}$, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=8.654859-2967.129 /\left(182.314+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $80.11-139.97^{\circ} \mathrm{C}$ (solid, Antoine eq., pressure gauge, Sasse et al. 1988)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=5.62672-1553.755 /\left(112.964+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $139.93-194.16^{\circ} \mathrm{C}$ (liquid, Antoine eq., pressure gauge, Sasse et al. 1988)
0.010, 0.014 (quoted $P_{L}$, supercooled liquid $P_{L}$, GC-RT correlation, Hinckley 1989)
$0.0158,0.0144 \quad$ (supercooled $P_{L}$, converted from literature $P_{S}$ with different $\Delta S_{\text {fus }}$ values, Hinckley et al. 1990)
$0.0113,0.00752 \quad\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=11.92-4104 /(\mathrm{T} / \mathrm{K})(\mathrm{GC}-\mathrm{RT}$ correlation, Hinckley et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=70.7671-6.9413 \times 10^{3} /(\mathrm{T} / \mathrm{K})-21.79 \cdot \log (\mathrm{~T} / \mathrm{K})+6.0727 \times 10^{-3} .(\mathrm{T} / \mathrm{K})+1.5767 \times 10^{-12} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 424-926 K (vapor pressure eq., Yaws 1994)
0.00446 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$0.000334-0.00306 ; 0.000601 ; 0.000293$ (quoted exptl.: effusion, gas saturation, manometry, Delle Site 1997)
$0.000173,0.00088 ; 0.000247,0.000572,0.000713$ (quoted lit., calculated; from GC-RT correlation, Delle Site 1997)
$0.00044^{*}$ (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range $35-125^{\circ} \mathrm{C}, \mathrm{Oja}$ \& Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=33.856-12400 /(\mathrm{T} / \mathrm{K})$; temp range $308-398 \mathrm{~K}$ (Clausius-Clapeyron eq., Knudsen effusion, Oja \& Suuberg 1998)
$1.51 \times 10^{-2} ; 1.94 \times 10^{-3}$
(quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.60-4263 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.49-3370 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$0.00073 \pm 0.00033$ (gas saturation-HPLC/fluorescence, de Seze et al. 2000)
$\log (\mathrm{P} / \mathrm{Pa})=12.748-4760.73 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol} 25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
1.89 (gas stripping, Southworth 1979)
$1.10 \quad$ (gas stripping, Mackay \& Shiu 1981)
1.21 (gas stripping-fluorescence, Shiu \& Mackay 1997)
2.0, 0.92 (gas stripping-HPLC/fluo., De Maagd et al. 1998)
0.496 (wetted wall column-GC, Altschuh et al. 1999)
1.71* (gas stripping-GC; measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-5159.97 /(\mathrm{T} / \mathrm{K})+10.103, \Delta \mathrm{H}=42.9 \mathrm{~kJ} \mathrm{~mol}^{-1}$, measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=9.17-2475 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
$4.90 \quad$ (calculated $-\pi$ const., Southworth et al. 1978)
5.32 (calculated-fragment const., Callahan et al. 1979)
4.88 (Hansch \& Leo 1979)
5.18 (shake flask-UV, concn. ratio, Karickhoff et al. 1979)
5.09 (shake flask-LSC, Means et al. 1979, 1980)
5.22 (calculated-f const., Yalkowsky \& Valvani 1980, Yalkowsky et al. 1983)
5.03 (HPLC-k' correlation, Hanai et al. 1981)
5.05 (HPLC-k' correlation, McDuffie 1981)
5.22 (RP-TLC-k' correlation, Bruggeman et al. 1982)
4.50 (HPLC-k' correlation, D'Amboise \& Hanai 1982)
4.88 (HPLC- $\mathrm{k}^{\prime}$ correlation, Hammers et al. 1982)
4.88 (HPLC-k' correlation, Hafkenscheid \& Tomlinson 1983)
4.96 (HPLC-RT correlation, Rapaport 1984)
5.52 (HPLC-RT/MS correlation, Burkhard et al. 1985)
4.80 (Hansch \& Leo 1985)
4.97 (RP-HPLC-RT correlation, Chin et al. 1986)
4.95 (Leo 1986)
$5.00 \pm 0.20$ (recommended, Sangster 1989, 1993)
4.88 (recommended, Hansch et al. 1995)
5.08; $5.39 \quad\left(26^{\circ} \mathrm{C} ; 4^{\circ} \mathrm{C}\right.$, Piatt et al. 1996)
$4.84 \pm 0.19,5.14 \pm 0.62 \quad$ (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
4.77
(shake flask-dialysis tubing-HPLC/UV, both phases, Andersson \& Schrăder 1999)
4.79
(shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section:

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8.60 (calculated- }\mp@subsup{\textrm{K}}{\textrm{OW}}{}/\mp@subsup{\textrm{K}}{\textrm{AW}}{}\mathrm{ , Wania & Mackay 1996)
8.61 (calculated, Finizio et al. 1997)
8.80*; 8.49 (generator column-GC; calculated-C }\mp@subsup{\textrm{C}}{\textrm{O}}{}/\mp@subsup{\textrm{C}}{\textrm{A}}{}\mathrm{ , measured range 0-40}\mp@subsup{}{}{\circ}\textrm{C}\mathrm{ , Harner & Bidleman 1998)
log K
8.75 (calculated-S Sot and vapor pressure P, Abraham et al. 2001)
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Bioconcentration Factor, $\log \mathrm{BCF}$ :

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3.43
    (Daphnia pulex, Southworth et al. 1978)
4.38 (mixed microbial population, Steen & Karickhoff 1981)
4.65 (P. hoyi, Eadie et al. 1982)
4.56, 4.22, 4.75 (average, Selenustrum capricornutum-dosed singly, dosed simultaneously, Casserly et al. 1983)
2.66 (goldfish, shake flask-GC, concn. ratio, Ogata et al. 1984)
3.43 (Daphnia pulex, Mackay & Hughes 1984)
3.43 (Daphnia magna, Newsted & Giesy 1987)
3.65, 3.81, 2.35 (mussel, clam, shrimp, Gobas & Mackay 1989)
2.85, 2.70
0.716, 1.124
    (Polychaete, Shrimo-hepatopancreas, Gobas & Mackay 1989)
    (Polychaete sp, Capitella capitata, Bayona et al. 1991)
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Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
4.92 (natural sediments, sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
4.81 (average value of soil and sediment, shake flask-LSC, sorption isotherms, Means et al. 1979)
4.92 (Kenaga \& Goring 1980)
4.80 (average value of 12 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1980)
4.78, 4.80 (soil/sediment: calculated- $\mathrm{K}_{\mathrm{OW}}$, regress of $\mathrm{K}_{\mathrm{P}}$ versus substrate properties, Means et al. 1980)
4.826 (sediment/soil, sorption isotherm by batch equilibrium technique, Karickhoff 1981)
3.11, 3.46 (sediment suspensions, Karickhoff \& Morris 1985)
5.23; 5.08 (fluorescence quenching interaction with AB humic acid; AB fulvic acid, Gauthier et al. 1986)
4.46-4.81; 4.94-5.51; 4.73-5.02 (marine humic acids; soil humic acids; soil fulvic acids, fluorescence quenching technique, Gauthier et al. 1987)
5.02 (dissolved humic materials, Aldrich humic acid, fluorescence quenching technique, Gauthier et al. 1987)
5.13 (sediment, batch equilibrium-GC, Vowles \& Mantoura 1987)
4.88 (soil-fine sand $0.2 \%$ OC, dynamic soil column studies, Enfield et al. 1989)
5.65 (LSC, Eadie et al. 1990)
6.51 (sediments average, Kayal \& Connell 1990)
4.83 (RP-HPLC-RT correlation, Pussemier et al. 1990)
4.82, 4.77 (RP-HPLC-RT correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
6.50 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
$5.05,5.00,4.88 ; 4.71$ (marine porewater organic colloids: Fort Point Channel FPC 7-9 cm, FPC 15-17 cm, FPC $25-29 \mathrm{~cm}$; Spectacle Island $14-16 \mathrm{~cm}$, Chin \& Gschwend 1992)
5.20, 5.18, 4.99; 5.23 (marine sediments: Fort Point Channel FPC 7-9 cm, FPC 15-17 cm, FPC 25-29 cm; Spectacle Island $14-16 \mathrm{~cm}$, Chin \& Gschwend 1992)
$4.78 ; 4.78,4.78$ (sediment: conen ratio $\mathrm{C}_{\text {sed }} / \mathrm{C}_{\mathrm{w}}$; conen-based coeff., area-based coeff. of flux studies of sediment/water boundary layer, Helmstetter \& Alden 1994)
5.50, 6.61, 6.06 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy \& Farrington 1995)
5.51, 5.34, 5.31; 7.43 (marine sediments: Fort Point Channel FPC 7-9 cm, FPC 15-17 cm, FPC 25-29 cm; Spectacle Island 14-16 cm, McGroddy \& Farrington 1995)
4.64 (Aldrich humic acid, Ozretich et al. 1995)
4.80, 4.81, 4.72 (RP-HPLC-k' correlation on different stationary phases, Szabo et al. 1995)
4.81 (range $4.73-4.66) ; 4.22$ (range $4.20-4.22)\left(4^{\circ} \mathrm{C}\right.$, low organic carbon sediment $\mathrm{f}_{\mathrm{OC}}=0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
4.62 (range 4.56-4.67); 4.0 (range 3.98-4.00) $\left(26^{\circ} \mathrm{C}\right.$, low organic carbon sediment $\mathrm{f}_{\mathrm{OC}}=0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
4.42-2.56 (5 soils, $20^{\circ} \mathrm{C}$, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
4.99, 4.98, 4.96, 4.97, 4.97 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choiu et al. 1998)
$5.14,5.22,5.23,5.12,5.04,5.24,5.45$; mean $4.98 \pm 0.009$ (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choiu et al. 1998)
3.47, 4.60, 3.53, 4.78, 4.61; mean $5.18 \pm 0.056$ (HPLC-screening method with different LC-columns, Szabo et al. 1999)
4.66, 4.78 (soils: organic carbon $\mathrm{OC} \geq 0.1 \%$, $\mathrm{OC} \geq 0.5 \%$, average, Delle Site 2001)
4.88, 4.90 (sediments: organic carbon $\mathrm{OC} \geq 0.1 \%, \mathrm{OC} \geq 0.5 \%$, average, Delle Site 2001)
5.47-6.68; 4.60-6.80 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
5.90 ; $5.89,5.60,5.56\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)
4.96; 4.70; 4.46-5.74 (calculated- $\mathrm{K}_{\mathrm{OW}}$; calculated-solubility; quoted lit. range, Schlautman \& Morgan 1993a)
4.50 at $\mathrm{pH} 4,4.37$ at $\mathrm{pH} 7,4.33$ at pH 10 in $0.001 \mathrm{M} \mathrm{NaCl} ; 4.35$ at $\mathrm{pH} 4,4.20$ at $\mathrm{pH} 7,4.245$ at pH 10 in 0.01 M $\mathrm{NaCl} ; 4.35$ at $\mathrm{pH} 4,4.15$ at $\mathrm{pH} 7,4.15$ at pH 10 in $0.1 \mathrm{M} \mathrm{NaCl} ; 4.33$ at $\mathrm{pH} 4,4.29$ at $\mathrm{pH} 7,4.15$ at pH 10 in $1 \mathrm{mM} \mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautmam \& Morgan 1993a)
4.19 at $\mathrm{pH} 4,3.89$ at $\mathrm{pH} 7,3.92$ at pH 10 in $0.001 \mathrm{M} \mathrm{NaCl} ; 4.15$ at $\mathrm{pH} 4,3.88$ at $\mathrm{pH} 7,3.86$ at pH 10 in 0.01 M NaCl ; 4.08 at $\mathrm{pH} 4,3.81$ at $\mathrm{pH} 7,3.785$ at pH 10 in $0.1 \mathrm{M} \mathrm{NaCl} ; 4.08$ at $\mathrm{pH} 4,3.90$ at $\mathrm{pH} 7,4.06$ at pH 10 in 1 mM $\mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautmam \& Morgan 1993a)
5.52 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)
4.66 (Askov soil, a Danish agriculture soil, Sverdrup et al. 2002)
5.35-6.33 (field contaminated sediment, initial-final values of 5-100 d contact time, gas-purge techniqueHPLC/fluorescence, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: sublimation rate constant of $1.1 \times 10^{-4} \mathrm{~s}^{-1}$ was measured as loss from glass surface at $24^{\circ} \mathrm{C}$ at an air flow rate of $3 \mathrm{~L} / \mathrm{min}$ (Cope \& Kalkwarf 1987)
Photolysis: calculated $t_{1 / 2}=4.2 \mathrm{~d}$ for direct sunlight photolysis in midday of midsummer at $40^{\circ} \mathrm{N}$ for inland water, and $\mathrm{t}_{1 / 2}=5.9 \mathrm{~d}$ for inland water with sediment partitioning (Zepp \& Schlotzhauer 1979)
$\mathrm{k}=1.014 \mathrm{~h}^{-1}$ (Zepp 1980)
$\mathrm{t}_{1 / 2}=0.68 \mathrm{hm}$ atmospheric and aqueous photolysis half-life, based on measured aqueous photolysis quantum yields calculated for midday summer sunlight at $40^{\circ} \mathrm{N}$ latitude (Zepp \& Schlotzhauer 1979; quoted, Harris 1982; Howard et al. 1991) and $t_{1 / 2}=2.04 \mathrm{~h}$ after adjusting for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
half-lives: $t_{1 / 2}=21 \mathrm{~h}$ on silica gel, $t_{1 / 2}=31 \mathrm{~h}$ on alumina and $t_{1 / 2}=46 \mathrm{~h}$ on fly ash on different atmospheric particulate substrates (approximate $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate) (Behymer \& Hites 1985);
$t_{1 / 2}=4.2 \mathrm{~d}$ for summer sunlight photolysis in surface water (Mill \& Mabey 1995)
$\mathrm{k}<1.05 \times 10^{-4} \mathrm{~m} / \mathrm{s}$ at $24^{\circ} \mathrm{C}$ with $\left[\mathrm{O}_{3}\right]=0.16 \mathrm{ppm}$ and light intensity of $1.3 \mathrm{~kW} / \mathrm{m}^{2}$ on glass surface of(Cope \& Kalkwarf 1987)
photodegradation $t_{1 / 2}=1 \mathrm{~h}$ in summer to days in winter by sunlight for adsorption on airborne particulates (Valerio et al. 1991);
photolysis $\mathrm{t}_{1 / 2}=0.68 \mathrm{~h}$ in water, based on direct photolysis in sunlight at midday, midsummer, latitude $40^{\circ} \mathrm{N}$ (Zepp 1991)
$\mathrm{k}(\operatorname{exptl})=0.00362 \mathrm{~min}^{-1}$ for pseudo-first-order direct photolysis, with $\mathrm{t}_{1 / 2}=3.18 \mathrm{~h}$, and the predicted $\mathrm{k}(\mathrm{calc})$ $=0.00382 \mathrm{~min}^{-1}$ by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
$\mathrm{t}_{1 / 2}($ obs. $)=2.63 \mathrm{~h}, \mathrm{t}_{1 / 2}(\mathrm{calc})=2.56 \mathrm{~h}$ by QSPR in atmospheric aerosol (Chen et al. 2001);
$\mathrm{k}=(2.08 \pm 0.13) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(9.24 \pm 0.53) \mathrm{h}$ in diesel particulate matter, photochemical degradation under atmospheric conditions, $\mathrm{k}=(1.88 \pm 0.16) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(10.22 \pm 0.95) \mathrm{h}$ in diesel particulate matter/soil mixture, and $\mathrm{t}_{1 / 2}=0.80$ to 1.59 h in various soil components using a $900-\mathrm{W}$ photo-irradiator as light source; $\mathrm{k}=(2.61 \pm 0.53) \times 10^{-7} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(737.55 \pm 124.49) \mathrm{h}$ in diesel particulate matter using a 300 W light source (Matsuzawa et al. 2001)

Photodegradation $\mathrm{k}=3.9 \times 10^{-4} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{3}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$\mathrm{k}=5 \times 10^{8} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $2.2 \times 10^{4} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}=(3.4-5.3) \times 10^{4} \mathrm{dm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ over pH range $1-7$, with $\mathrm{t}_{1 / 2}=0.18 \mathrm{~s}$ in presence of $10^{-4} \mathrm{M}$ ozone at pH
7 for the reaction with $\mathrm{O}_{3}$ in water at $25^{\circ} \mathrm{C}$ (Butković et al. 1983)
$\mathrm{k}_{\mathrm{OH}}=5.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}} \approx-5.6 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1990)
photooxidation $\mathrm{t}_{1 / 2}=0.802-8.02 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation: significant degradation within 7 d for a domestic sewage 28 -d test for an average of three staticflask screening (Tabak et al. 1981)
$\mathrm{t}_{1 / 2}($ aq. aerobic $)=5040-45600 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; Sims 1990; quoted, Howard et al. 1991)
$\mathrm{k}=0.29 \mathrm{~h}^{-1}$ in atmosphere (Dragoscu \& Friedlander 1989; quoted, Tsai et al. 1991)
$\mathrm{k}=0.0027 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=260 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0035 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=199 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
$\mathrm{t}_{1 / 2}($ anaerobic $)=20160-182400 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation halflife (Howard et al. 1991).
Biotransformation: estimated to be $1 \times 10^{-10} \mathrm{~mL}^{\text {cell }}{ }^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982)
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=1126 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.343 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)
$\log \mathrm{k}_{1}=3.05 \mathrm{~h}^{-1} ; \log \mathrm{k}_{2}=-0.46 \mathrm{~h}^{-1}$ (Daphnia pulex, correlated as per Mackay \& Hughes 1984, Hawker \& Connell 1986)
$\mathrm{k}_{1}=113.0 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.017 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, S. heringianus, Frank et al. 1986)
$\mathrm{k}_{2}=0.017 \mathrm{~h}^{-1}$ (S. heringianus, Frank et al. 1986)
$\mathrm{k}_{1}=199.2 \mathrm{~mL} \mathrm{~g}^{-1} \cdot \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0012 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}, P\right.$. hoyi, Landrum 1988)
$\mathrm{k}_{1}=3.4-5.3 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.022 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.68-2.04 \mathrm{~h}$, based on estimated sunlight photolysis half-life in water (Zepp \& Stotzhauer 1979; Lyman et al. 1982; quoted, Howard et al. 1991);
half-lives under simulated atmospheric conditions: $\mathrm{t}_{1 / 2}=4.20 \mathrm{~h}$ under simulated sunlight, $\mathrm{t}_{1 / 2}=2.75 \mathrm{~h}$ under simulated sunlight + ozone ( 0.2 ppm ), $\mathrm{t}_{1 / 2}=15.72 \mathrm{~h}$ under dark reaction ozone ( 0.2 ppm ) (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983);
$\mathrm{t}_{1 / 2}=2.5 \mathrm{~h}$ with a steady-state concn of tropospheric ozone of $2 \times 10^{-9} \mathrm{M}$ in clean air (Butković et al. 1983);
photooxidation $\mathrm{t}_{1 / 2}=0.802-8.02 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: computed near-surface $t_{1 / 2}=0.58 \mathrm{~h}$ for direct photochemical transformation at latitude $40^{\circ} \mathrm{N}$, midday, midsummer, $\mathrm{t}_{1 / 2}=4.2 \mathrm{~h}$ for direct photolysis in a $5-\mathrm{m}$ deep inland water body with no sedimentwater partitioning and $\mathrm{t}_{1 / 2}=5.9 \mathrm{~d}$ with sediment-water partitioning (Zepp \& Schlotzhauer 1979);
$t_{1 / 2}=0.68-2.04 \mathrm{~h}$, based on estimated sunlight photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}=1.8 \mathrm{~s}$ in presence of $10^{-4} \mathrm{M}$ ozone at pH 7 (Butković et al. 1983);
$\mathrm{t}_{1 / 2}=4.2 \mathrm{~d}$ for summer at $40^{\circ} \mathrm{N}$ latitude under sunlight (Mill \& Mabey 1985);
$\mathrm{t}_{1 / 2}=0.68 \mathrm{~h}$, based on direct photolysis in sunlight at midday, mid-summer and $40^{\circ} \mathrm{N}$ latitude (quoted, Zepp 1991);
photolysis $\mathrm{t}_{1 / 2}=3.18 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp
(Chen et al. 1996).
Groundwater: $\mathrm{t}_{1 / 2}=10080-91200 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: reduction $t_{1 / 2}=547 \mathrm{~h}$ for chemical available pyrene and $\mathrm{t}_{1 / 2}=298 \mathrm{~h}$ for bioavailable pyrene for amphipod, P. hoyi in Lake Michigan sediments at $4^{\circ} \mathrm{C}$. The uptake clearance from sediment, $\mathrm{k}=(0.019-0.015) \mathrm{g}$ of dry sediment $\cdot \mathrm{g}^{-1}$ of organism $\cdot \mathrm{h}^{-1}$, and the rate constants to become biologically unavailable were $\mathrm{k}=0.0019$
$\mathrm{h}^{-1}$ for 10 -d aged sediment corresponding to $\mathrm{a}_{1 / 2}=365 \mathrm{~d}$ and $\mathrm{k}=0.0030 \mathrm{~h}^{-1}$ for nonaged sediment corresponding to a $t_{1 / 2}=231 \mathrm{~h}$ (Landrum 1989).
Soil: $\mathrm{t}_{1 / 2}=3-35 \mathrm{~h}$ (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$\mathrm{t}_{1 / 2}=58 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and $\mathrm{t}_{1 / 2}=48 \mathrm{~d}$ for $50 \mathrm{mg} / \mathrm{kg}$ treatment (Bulman et al. 1987);
$\mathrm{t}_{1 / 2}=5040-45600 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; Sims 1990; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
degradation rate constant, $\mathrm{k}=0.0027 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=260 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{k}=0.0035 \mathrm{~d}^{-1}$ with $t_{1 / 2}=199 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$\mathrm{t}_{1 / 2}=500 \mathrm{~d}$ in soil (Jury et al. 1990);
$\mathrm{t}_{1 / 2}=0.4$ to more than $90 \mathrm{wk}, 8.5 \mathrm{yr}$ (quoted, Luddington soil, Wild et al. 1991).
Biota: depuration $\mathrm{t}_{1 / 2}=40.8 \mathrm{~h}$ in $s$. heringianus (Frank et al. 1986);
elimination $\mathrm{t}_{1 / 2}=4.1-5.5 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=10.3 \mathrm{~d}$ from clam Mya areneria, $\mathrm{t}_{1 / 2}=14.4 \mathrm{~d}$ from polychaete Abarenicola pacifica, $\mathrm{t}_{1 / 2}=6.7 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=0.80 \mathrm{~d}$ from shrimp, $\mathrm{t}_{1 / 2}=3.6 \mathrm{~d}$ from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.29.1
Reported aqueous solubilities of pyrene at various temperatures
1.

| Wauchope \& Getzen 1972 |  |  |  | Schwarz 1977 |  | May et al. 1978a |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| shake flask-UV |  |  |  | shake flask-fluorescence |  | generator column-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
|  | experimental |  | smoothed |  |  |  |  |
| 22.2 | 0.129 | 0 | 0.049 | 12.2 | 0.055 | 25 | 0.132 |
| 22.2 | 0.128 | 22.2 | 0.130 | 15.5 | 0.069 | 29 | 0.162 |
| 22.2 | 0.124 | 25 | 0.148 | 17.4 | 0.079 |  |  |
| 34.5 | 0.228 | 34.5 | 0.235 | 20.3 | 0.092 | temp dependence eq. 2 |  |
| 34.5 | 0.235 | 44.7 | 0.399 | 23.0 | 0.117 | S | $\mu \mathrm{g} / \mathrm{kg}$ |
| 44.7 | 0.397 | 50 | 0.532 | 23.3 | 0.118 | a | -0.0011 |
| 44.7 | 0.395 | 50.1 | 0.534 | 25.0 | 0.129 | b | 0.2007 |
| 44.7 | 0.405 | 55.6 | 0.730 | 26.2 | 0.144 | c | -1.051 |
| 50.1 | 0.558 | 56.0 | 0.74 | 26.7 | 0.145 | d | 50.2 |
| 50.1 | 0.576 | 60.7 | 0.97 | 28.5 | 0.164 |  |  |
| 50.1 | 0.556 | 65.2 | 1.27 | 31.3 | 0.188 | $\Delta \mathrm{H}_{\text {sol }} /$ / k | $=35.44$ |
| 55.6 | 0.75 | 71.9 | 1.90 |  |  | for tem | $5-30^{\circ} \mathrm{C}$ |
| 55.6 | 0.75 | 74.7 | 2.26 | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=47.70$ |  |  |  |
| 55.6 | 0.77 | 75.0 | 2.31 |  |  |  |  |
| 56.0 | 0.74 |  |  |  |  |  |  |
| 60.7 | 0.96 | temp dependence eq. 1 |  |  |  |  |  |
| 60.7 | 0.95 | $\ln x$ | mole fraction |  |  |  |  |
| 60.7 | 0.90 | $\Delta \mathrm{H}_{\text {fus }}$ | $15.3 \pm 0.084$ |  |  |  |  |
| 65.2 | 1.27 | $10^{2} \cdot \mathrm{~b}$ | $4.78 \pm 0.09$ |  |  |  |  |
| 65.2 | 1.29 | c | $38.1 \pm 0.3$ |  |  |  |  |
| 71.9 | 1.83 |  |  |  |  |  |  |
| 71.9 | 1.86 |  |  |  |  |  |  |
| 71.9 | 1.89 |  |  |  |  |  |  |
| 74.7 | 2.21 |  |  |  |  |  |  |
| $\Delta \mathrm{H}_{\text {fus }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=15.3$ |  |  |  |  |  |  |  |

Empirical temperature dependence equations:
Wauchope \& Getzen (1972): R•ln $x=-\left[\mathrm{H}_{\mathrm{fus}} /(\mathrm{T} / \mathrm{K})\right]+(0.000408)[(\mathrm{T} / \mathrm{K})-291.15]^{2}-\mathrm{c}+\mathrm{b} \cdot(\mathrm{T} / \mathrm{K})$
May et al. (1978):- $\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}$

TABLE 4.1.1.29.1 (Continued)
2.

| May 1980 |  | May et al. 1983 |  | Shaw 1989 |  | Reza et al. 2002 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| generator column-HPLC |  | generator column-HPLC |  | IUPAC recommended |  | generator column- <br> HPLC/fluo |  |
| ${ }^{1} /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 4.7 | 0.0492 | 4.7 | 0.0492 | 0 | 0.050 | 8.54 | 0.0474 |
| 9.5 | 0.0585 | 9.5 | 0.0586 | 20 | 0.090 | 10.39 | 0.0566 |
| 14.3 | 0.0720 | 14.3 | 0.0721 | 25 | 0.132 | 13.5 | 0.0635 |
| 18.7 | 0.0933 | 18.7 | 0.0934 | 30 | 0.175 | 14.46 | 0.0694 |
| 21.2 | 0.109 | 21.2 | 0.1091 | 40 | 0.30 | 15.7 | 0.0804 |
| 25.5 | 0.136 | 25.5 | 0.1361 | 50 | 0.50 | 18.05 | 0.0871 |
| 29.9 | 0.170 | 29.9 | 0.1701 | 60 | 0.90 | 21.53 | 0.1087 |
|  |  |  |  | 70 | 1.70 | 25.55 | 0.1331 |
| temp dependence eq. 2 |  |  |  | 75 | 2.30 | 27.36 | 0.1505 |
| S | $\mu \mathrm{g} / \mathrm{kg}$ |  |  |  |  | 29.66 | 0.1686 |
| a | -0.0011 |  |  |  |  | 21.28 | 0.1931 |
| b | 0.2007 |  |  |  |  |  |  |
| c | -1.051 |  |  |  |  | $\ln x=$ | /T(K) |
| d | 50.2 |  |  |  |  | A | -1.30 |
|  |  |  |  |  |  | B | 5059 |
| $\begin{aligned} & \Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=35.44 \\ & \text { for temp range } 5-30^{\circ} \mathrm{C} \end{aligned}$ |  |  |  |  |  | temp ran | -305 K |



FIGURE 4.1.1.29.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for pyrene.

TABLE 4.1.1.29.2
Reported vapor pressures of pyrene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log P=A-B /(C+T / K)$
$\log P=A-B /(T / K)-C \cdot \log (T / K)$
1.


|  |  |
| ---: | ---: | ---: |
| $\mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=93.90$ | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=101.04$ |
| at 298.15 K |  |

2. 

| Smith et al. 1980 |  | Sonnefeld et al. 1983 |  | Sasse et al. 1988 |  | Oja \& Suuberg 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| inclined-piston gauge |  | gas saturation-HPLC |  | electronic manometry |  | Knudsen effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
|  | solid |  |  | solid |  |  |  |
| 125 | 12.4 | 10.5 | $9.20 \times 10^{-5}$ | 80.11 | 0.30 | 46.95 | 0.00863 |
| 130 | 17.5 | 10.5 | $9.21 \times 10^{-5}$ | 90.10 | 0.764 | 56.99 | 0.0243 |
| 135 | 24.7 | 10.5 | $9.53 \times 10^{-5}$ | 100.11 | 1.853 | 37.98 | 0.0209 |
| 140 | 34.7 | 20.9 | $3.35 \times 10^{-4}$ | 110.14 | 4.360 | 68.03 | 0.0852 |
| 145 | 48.0 | 20.9 | $3.35 \times 10^{-4}$ | 120.08 | 9.213 | 72.99 | 0.164 |
| 149 | 62.1 | 20.9 | $3.39 \times 10^{-4}$ | 120.10 | 9.40 | 83.99 | 0.428 |
| 150 | 66.1 | 30.0 | $1.10 \times 10^{-4}$ | 129.99 | 19.20 | 93.02 | 0.945 |
|  | liquid | 30.0 | $1.09 \times 10^{-4}$ | 134.98 | 26.80 |  |  |
| 125 | 17.1* | 30.0 | $1.03 \times 10^{-4}$ | 139.97 | 37.07 | eq. 1a | $\mathrm{P} / \mathrm{Pa}$ |
| 130 | 22.5* | 39.34 | $3.31 \times 10^{-3}$ | liquid |  | A | 33.856 |
| 135 | 29.9* | 39.34 | $3.47 \times 10^{-3}$ | 139.93 | 40.80 | B | 12400 |
| 140 | 39.5* | 39.34 | $3.25 \times 10^{-3}$ | 144.90 | 53.06 |  |  |
| 145 | 51.3* | 39.45 | $3.41 \times 10^{-3}$ | 149.82 | 68.66 | $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ}$ | $=103.10$ |

## TABLE 4.1.1.29.2 (Continued)

2. 

| Smith et al. 1980 |  | Sonnefeld et al. 1983 |  | Sasse et al. 1988 |  | Oja \& Suuberg 1998 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| inclined-piston gauge |  | gas saturation-HPLC |  | electronic manometry |  | Knudsen effusion |  |
| $t^{\circ} \mathrm{C}$ | $\mathbf{P} / \mathbf{P a}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | $\mathrm{t}^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |
| 149 | 63.3* | 39.45 | $3.20 \times 10^{-3}$ | 159.75 | 112.5 |  |  |
| 150 | 66.7* | 25.0 | $6.0 \times 10^{-4}$ | 169.61 | 178.8 |  |  |
| 152 | 78.3 |  |  | 179.45 | 279.4 |  |  |
| 155 | 86.5 | eq. 2 | P/Pa | 189.25 | 405.7 |  |  |
| 160 | 110.7 | A | 12.748 | 194.16 | 490.1 |  |  |
| 165 | 141.6 | B | 4760.73 |  |  |  |  |
| 170 | 178.9 | temp ra | $10-50^{\circ} \mathrm{C}$ | for solid |  |  |  |
| 175 | 224.6 |  |  | eq. 2 | P/mmHg |  |  |
| 180 | 280.4 | $\Delta \mathrm{H}_{\text {subl }} /(\mathrm{kJ}$ | $\left.\mathrm{l}^{-1}\right)=91.20$ | A | 8.654859 |  |  |
| 185 | 345.3 |  | B | 2967.129 |  |  |  |
|  |  |  |  | C | 182,314 |  |  |
| *supercooled liquid values |  |  |  | temp range: | 1-139.97 ${ }^{\circ} \mathrm{C}$ |  |  |
|  |  |  |  | $\Delta \mathrm{H}_{\text {subl }} /(\mathrm{kJ}$ | -1) $=97.70$ |  |  |
| reported vapor pressure eq. see foot note |  |  |  |  |  |  |  |
|  |  |  | eq. 2 | $\underset{\mathrm{A}}{\mathrm{P} / \mathrm{mmHg}}$ | 5.62672 |  |  |
| $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=103.9$ |  |  | B | 1553.755 |  |  |  |
|  |  |  |  | C | 112.964 |  |  |
|  |  |  |  | temp range | $\text { 7. } 97-194^{\circ} \mathrm{C}$ |  |  |

[^2]

FIGURE 4.1.1.29.2 Logarithm of vapor pressure versus reciprocal temperature for pyrene.

TABLE 4.1.1.29.3
Reported Henry's law constants and octanol-air partition coefficients of pyrene at various temperatures and temperature dependence equations

| Henry's law constant |  |  | $\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {OA }}$ |  |
| :---: | :---: | :---: | :---: | :---: |
| Bamford et al. 1999 |  |  | Harner \& Bidleman 1998 |  |
| gas stripping-GC/MS |  |  | generator column-GC/FID |  |
| t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | H/(Pa m$\left.{ }^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | $\log K_{\text {OA }}$ |
|  |  | average |  |  |
| 4.1 | 0.37, 0.49 | 0.43 | 0 | 9.966 |
| 11.0 | 0.63, 0.76 | 0.69 | 10 | 9.528 |
| 18.0 | 1.02, 1.19 | 1.10 | 20 | 9.155 |
| 25.0 | 1.54, 1.89 | 1.71 | 30 | 8.647 |
| 31.0 | 2.15, 2.80 | 2.45 | 40 | 8.121 |
|  |  |  | 25(exptl) | 8.80 |
| $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  | 25(calc) | 8.49 |
| A | 10.1034 |  |  |  |
| B | 5160 |  | $\log \mathrm{K}_{\mathrm{OA}}=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
|  |  |  | A | -4.56 |
| enthalpy, entropy change: |  |  | B | 3985 |
| $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=42.9 \pm 2.3$ |  |  |  |  |
| $\Delta \mathrm{S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=84$ |  |  | enthalpy of phase change |  |
|  | at $25^{\circ} \mathrm{C}$ |  | $\Delta \mathrm{H}_{\mathrm{OA}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=76.3$ |  |



FIGURE 4.1.1.29.3 Logarithm of Henry's law constant and $K_{O A}$ versus reciprocal temperature for pyrene.

### 4.1.1.30 Fluoranthene



Common Name: Fluoranthene
Synonym: idryl, 1,2-benzacenaphthene, benzo[j,k]fluorene, benz[a]acenaphthylene, fluoranthrene
Chemical Name: 1,2-benzacenaphthene
CAS Registry No: 206-44-0
Molecular Formula: $\mathrm{C}_{16} \mathrm{H}_{10}$
Molecular Weight: 202.250
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
110.19 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
384 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
$1.252\left(0^{\circ} \mathrm{C}\right.$, Weast 1982-83, Dean 1985; Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
162 (calculated-density, liquid molar volume, Lande \& Banerjee 1981)
217.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
18.87 (Ruelle \& Kesselring 1997)
18.74 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
49.37 (Casellato et al. 1973; quoted, Yalkowsky 1981)
47.70 (differential scanning calorimetry, Hinckley et al. 1990)
48.89, 36.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999) 49.6 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.146 ( mp at $110.19^{\circ} \mathrm{C}$ )
0.191 (calculated, $\Delta \mathrm{S}_{\text {fus }}=49.6 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.240 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.265 (shake flask-UV, Klevens 1950)
$0.240 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
0.236 (fluorescence/UV, Schwarz \& Wasik 1976)
0.260 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.206 (Rossi 1977; Neff 1979)
0.206* (generator column-HPLC/UV, measured range 8.1-29.9 ${ }^{\circ} \mathrm{C}$, May et al. 1978a,b)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=50.4+4.322 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)-0.1047 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0072 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$; temp range $5-30^{\circ} \mathrm{C}$ (generator column-
HPLC/UC, May et al. 1978b)
0.120 (shake flask-nephelometry, Hollifield 1979)
0.218 (OECD 1979/1980; quoted, He et al. 1995)
$0.275,0.373\left(15,25^{\circ} \mathrm{C}\right.$, generator column/elution method, average values of 6-7 laboratories, OECD 1981)
$0.200 \quad\left(20^{\circ} \mathrm{C}\right.$, quoted, Schmidt-Bleek et al. 1982)
$0.190 \quad\left(20^{\circ} \mathrm{C}\right.$, generator column-fluorescence, Hashimoto et al. 1982)
0.203* $\quad\left(24.6^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range $281.25-303.05 \mathrm{~K}$, May et al. 1983)
0.243 (average lit. value, Pearlman et al. 1984)
0.199 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
1.43 (RP-HPLC-RT correlation, Chin et al. 1986)
0.283 (vapor saturation-UV, Akiyoshi et al. 1987)
0.240 (recommended, Shaw 1989)
0.222 (generator column-HPLC/fluorescence, Kishi \& Hashimoto 1989)
0.373 (average value of Japan, OECD tests, Kishi \& Hashimoto 1989)
0.166 (shake flask-fluorescence, Kishi \& Hashimoto 1989)
0.265 (shake flask-HPLC/UV/fluorescence, Pinal et al. 1991)
0.177 (generator column-HPLC, Vadas et al. 1991)
0.248 (generator column-HPLC/UV, Yu \& Xu 1993)
0.207 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
$0.2289 \pm 0.0008 \quad$ (shake flask-SPME (solid-phase micro-extraction)-GC, Paschke et al. 1999)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=0.779-987.5 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=-1.796327-4772.17 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$653^{*} \quad\left(197.0^{\circ} \mathrm{C}\right.$, temp range $197.0-384.2^{\circ} \mathrm{C}$, Tsypkina 1955 ; quoted, Boublik et al. 1984)
$6.67 \times 10^{-4} \quad$ (effusion method, Hoyer \& Peperle 1958)
$\log (\mathrm{P} / \mathrm{mmHg})=12.67-5357 /(\mathrm{T} / \mathrm{K})$; temp range $25-85^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958)
0.00123* (gas saturation-HPLC/fluo.or UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=11.901-4416.56 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (Antoine eq., gas saturation, Sonnefeld et al. 1983)
0.00124 (generator column-HPLC/fluo., Wasik et al. 1983)
1.79 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, extrapolated from Antoine eq., Boublik et al. 1984)
$0.0154,0.0067$ ( $\mathrm{P}_{\mathrm{GC}}$ by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
$0.00861 \quad$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with $\Delta \mathrm{S}_{\text {fus }}$ Bidleman 1984)
0.000125 (extrapolated-Antoine eq., Boublik et al. 1984)
$\log (\mathrm{P} / \mathrm{kPa})=5.45017-1717.489 /\left(114.025+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$; temp range $197-384.2^{\circ} \mathrm{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)
$1.65 \times 10^{-4}$ (extrapolated, Antoine eq., Dean 1985, 1992)
$\log (\mathrm{P} / \mathrm{mmHg})=6.373-1756 /\left(118+\mathrm{t} /{ }^{\circ} \mathrm{C}\right) 1$;temp range $197-384^{\circ} \mathrm{C}$ (Antoine eq., Dean 1985, 1992)
0.00105 (extrapolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.96071-5348.06 /(\mathrm{T} / \mathrm{K})$; temp range $298-383 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.67549-2957.01 /(-24.15+\mathrm{T} / \mathrm{K})$; temp range $503-658 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$0.00068,0.0056$ (lit. solid $\mathrm{P}_{\mathrm{S}}$, supercooled liquid $\mathrm{P}_{\mathrm{L}}$, Bidleman \& Foreman 1987)
0.992 (WERL Treatability database, quoted, Ryan et al. 1988)
$0.00861,0.00635$ (supercooled $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with different $\Delta \mathrm{S}_{\text {fus }}$ values, Hinckley et al. 1990)
$0.0155,0.00955\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=11.35-4040 /(\mathrm{T} / \mathrm{K})(\mathrm{GC}-\mathrm{RT}$ correlation, Hinckley et al. 1990)
$\log (\mathrm{P} / \mathrm{mmHg})=70.6802-6.484 \times 10^{3} /(\mathrm{T} / \mathrm{K})-22.241 \cdot \log (\mathrm{~T} / \mathrm{K})+7.2184 \times 10^{-3} \cdot(\mathrm{~T} / \mathrm{K})-6.3035 \times 10^{-13} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 383-905 K (vapor pressure eq., Yaws 1994)
0.00692 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$0.00168,0.000672 ; 0.00124$ (quoted exptl. values, effusion; gas saturation, Delle Site 1997)
$0.00218,0.000939,0.000889$ (quoted lit. values, from GC-RT correlation, Delle Site 1997)
$7.48 \times 10^{-3} ; 1.43 \times 10^{-3}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990 ; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.62-4310 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.03-3323 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{Pa})=11.901-4415.56 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
0.00598 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4141 /(\mathrm{T} / \mathrm{K})+11.66 ; \Delta \mathrm{H}_{\text {vap }}=-79.3 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol} 25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.65* (gas stripping-HPLC/fluorescence, measured range $10-55^{\circ} \mathrm{C}$, ten Hulscher et al. 1992)
1.10 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)
1.96* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-4654.8 /(\mathrm{T} / \mathrm{K})+8.42, \Delta \mathrm{H}=38.7 \mathrm{~kJ} \mathrm{~mol}^{-1}$; measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log [\mathrm{H} /(\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol})]=8.23-2336 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
1.96 (quoted from Bamford et al. 1999; Dachs \& Eisenreich 2000)
$0.602\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured values, Staudinger \& Robers 1996 , 2001) $\log \mathrm{K}_{\mathrm{AW}}=6.175-2868 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :

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5.22 (RP-TLC- \(\mathrm{k}^{\prime}\) correlation, Bruggeman et al. 1982)
4.47 (HPLC-k' correlation, Harnisch et al. 1983)
4.84 (RP-HPLC-RT correlation, Chin et al. 1986)
4.85 (HPLC-RT correlation, Wang et al. 1986)
5.16 (shake flask/slow stirring-GC, De Bruijn et al. 1989)
\(5.20 \quad\) (recommended, Sangster 1989, 1993)
5.17 (TLC-RT correlation, De Voogt et al. 1990)
\(5.148 \pm 0.077,5.155 \pm 0.015\) (shake flask/slow stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)
5.00 (shake flask-UV spec., Alcorn et al. 1993)
5.16 (recommended, Hansch et al. 1995)
5.23 (5.12-5.31) (shake flask/slow stirring-HPLC/fluorescence., De Maagd et al. 1998)
5.16 (shake flask-SPME solid-phase micro-extraction; Paschke et al. 1999)
\(0.602 \quad\left(20^{\circ} \mathrm{C}\right.\), selected from literature experimentally measured data, Staudinger \& Roberts 2001)
\(\log \mathrm{K}_{\mathrm{AW}}=5.485-2682 /(\mathrm{T} / \mathrm{K})\), (van’t Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
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Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section:
8.60 (calculated- $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, Wania \& Mackay 1996)
8.60 (calculated, Finizio et al. 1997)
$8.80^{*} ; 8.60$ (generator column-GC; calculated- $\mathrm{C}_{\mathrm{O}} / \mathrm{C}_{\mathrm{A}}$, measured range $0-40^{\circ} \mathrm{C}$, Harner \& Bidleman 1998) $\log \mathrm{K}_{\mathrm{OA}}=-5.94+4417 /(\mathrm{T} / \mathrm{K})$; temp range $20-40^{\circ} \mathrm{C}$ (generator column-GC, Harner \& Bidleman 1998)
8.61 (calculated- $\mathrm{S}_{\text {oct }}$ and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log$ BCF:
3.18 (calculated as per Kenaga \& Goring 1979, Eadie et al. 1982)
$4.90 \quad$ (P. hoyi, Eadie et al. 1982)
4.08 (microorganisms-water, calculated from $\mathrm{K}_{\mathrm{OW}}$, Mabey et al. 1982)
3.24 (Daphnia magna, Newsted \& Giesy 1987)
0.756, 1.079 (Polychaete sp, Capitella capitata, Bayona et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
6.38 (sediments average, Kayal \& Connell 1990)
4.74, 4.62 (RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)
6.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
4.816; 4.81, 4.82 (sediment: conen ratio $\mathrm{C}_{\text {sed }} / \mathrm{C}_{\mathrm{w}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter \& Alden 1994)
4.51, 5.05, 4.16 (sediments from Brown's Lake, Hamlet City Lake, WES reference soil, shake flask-LSC, Brannon et al. 1995)
6.56, 6.66, 6.08 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy \& Farrington 1995)
4.62 (calculated-MCI ${ }^{1} \chi$, Sabljic et al. 1995)
$5.25\left(10^{\circ} \mathrm{C}\right), 5.22,5.12\left(20^{\circ} \mathrm{C}\right), 5.05\left(35^{\circ} \mathrm{C}\right), 4.89,4.96\left(45^{\circ} \mathrm{C}\right)\left(\log \mathrm{K}_{\mathrm{DOC}}\right.$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers \& ten Hulscher 1996)
$5.40 \quad\left(20^{\circ} \mathrm{C}, \log \mathrm{K}_{\mathrm{POC}}-\right.$ particulate organic material from lake, Lüers \& ten Hulscher 1996)
$4.81,4.65,4.80,4.82 ; 4.813 ; 4.727$ ( 4 soils with different organic carbon content $\mathrm{f}_{\mathrm{OC}}$, adsorption equilibriumshake flask-HPLC; calculated- $\mathrm{K}_{\text {Ow }}$; calculated-S, He et al. 1996)
5.32 (5.29-5.35), 4.89 (4.89-4.90) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flaskHPLC/UV, de Maagd et al. 1998)
4.62, 4.03; 3.40, 4.49, 3.55, 4.53, 4.56 (quoted lit., calculated- $\mathrm{K}_{\mathrm{Ow}}$; HPLC-screening method with different LCcolumns, Szabo et al. 1999)
5.32-6.59; 4.60-6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$5.83 ; 6.79,5.53,5.52\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)
4.91, 4.65 (average values for sediments, soils, organic carbon OC $\geq 0.5 \%$, Delle Site 2001)
4.62 (Askov soil, a Danish agricultural soil, Sverdrup et al. 2002)
5.21-6.60 (field contaminated sediment, initial-final values of 5-100 d contact time, gas-purge techniqueHPLC/fluorescence, ten Hulscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: direct photochemical transformation $\mathrm{t}_{1 / 2}($ calc $)=21 \mathrm{~h}$, computed near-surface water, latitude $40^{\circ} \mathrm{N}$, midday, midsummer and photolysis $\mathrm{t}_{1 / 2}=160 \mathrm{~d}$ and 200 d in $5-\mathrm{m}$ deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, $40^{\circ} \mathrm{N}$ (Zepp \& Schlotzhauer 1979) $t_{1 / 2}=21 \mathrm{~h}$, atmospheric and aqueous photolysis half life, based on measured sunlight photolysis rate constant in water adjusted for midday summer sunlight at $40^{\circ} \mathrm{N}$ latitude and $\mathrm{t}_{1 / 2}=63 \mathrm{~h}$ after adjusting for approximate winter sunlight intensity (Howard et al. 1991);
$t_{1 / 2}=160 \mathrm{~d}$ under summer sunlight in surface water (Mill \& Mabey 1985);
half-lives on different atmospheric particulate substrates (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=74 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=23 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=44 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985);
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{obs})=.3.61 \mathrm{~h}, \mathrm{t}_{1 / 2}(\mathrm{calc})=4.78 \mathrm{~h}$, by QSPR in atmospheric aerosol (Chen et al. 2001); $\mathrm{k}=(1.76 \pm 0.13) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(10.93 \pm 0.75) \mathrm{h}$ in diesel particulate matter, photochemical degradation under atmospheric conditions, $\mathrm{k}=(2.97 \pm 0.40) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(6.48 \pm 1.03) \mathrm{h}$ in diesel particulate matter/soil mixture, and $t_{1 / 2}=1.6$ to 4.15 h in various soil components using a $900-\mathrm{W}$ photo-irradiator as light source; $\mathrm{k}=(8.69 \pm 0.29) \times 10^{-6} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(22.16 \pm 0.77) \mathrm{h}$ in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)
Photodegradation $\mathrm{k}=5.0 \times 10^{-6} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant, k , and for gas-phase second-order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$, or as indicated *data at other temperatures and/or the Arrhenius expression see reference:
k (calc) $<3600 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $<360 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}_{\mathrm{OH}}=5.0 \times 10^{-11} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ and $\mathrm{k}_{\mathrm{N}_{2} \mathrm{O}_{5}} \approx 1.8 \times 10^{-17} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ for reaction with $\mathrm{N}_{2} \mathrm{O}_{5}$ at $296 \pm 2 \mathrm{~K}$ (relative rate method, Atkinson et al. 1990)
photooxidation half-life of $2.02-20.2 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
$\mathrm{k}_{\mathrm{OH}}{ }^{*}=11 \times 10^{-12} \mathrm{~cm}^{3}$ molecule ${ }^{-1} \mathrm{~s}^{-1}$ at 298 K , measured range $306-366 \mathrm{~K}$ with a calculated atmospheric lifetime of 26 h based on gas-phase OH reactions (Brubaker \& Hites 1998)
Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation: aquatic $\mathrm{k}=2.2 \times 10^{-3} \mu \mathrm{~mol} \mathrm{~h}{ }^{-1} \mathrm{mg}^{-1}$ with bacterial protein (Barnsley 1975; quoted, Callahan et al. 1979)
significant with gradual degradation for a domestic sewer test for an average three static-flask screening (Tabak et al. 1981)
$\mathrm{t}_{1 / 2}($ aerobic $)=3360-10560 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; quoted, Howard et al. 1991)
$\mathrm{k}=0.19 \mathrm{~h}^{-1}$ in atmosphere (Dragoescu \& Friedlander 1989)
$\mathrm{k}=0.0018 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=377 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0026 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=268 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
$t_{1 / 2}($ anaerobic $)=13440-42240 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
first order $\mathrm{k}=0.132$ to $0.162 \mathrm{~L} \mathrm{mg}^{-1} \mathrm{~d}^{-1}$ for a marine PAH-degrading enrichment without sediment, the degradation rate was 2.1 to 5.3 times faster with sediment present (Poeton et al. 1999)
Biotransformation: estimated rate constant for bacteria, $1 \times 10^{-10} \mathrm{~mL}$ cell ${ }^{-1} \mathrm{~h}^{-1}$ (Mabey et al. 1982).
Bioconcentration, Uptake $\left(k_{1}\right)$ and Elimination $\left(k_{2}\right)$ Rate Constants:
$\mathrm{k}_{1}=4.1-6.1 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.026 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
$\mathrm{k}_{2}=0.15 \mathrm{~h}^{-1}$ in water with corresponding $\mathrm{t}_{1 / 2}=4.7 \mathrm{~h}$ and $\mathrm{k}_{2}=0.14 \mathrm{~h}^{-1}$ in sediment with corresponding $\mathrm{t}_{1 / 2}=$
4.9 h for copepods $S$. knabeni in 24-h experiments (Lotufo 1998)
$\mathrm{k}_{2}=0.17 \mathrm{~h}^{-1}$ in sediment with corresponding $\mathrm{t}_{1 / 2}=4.2 \mathrm{~h}$ and $\mathrm{k}_{2}=0.09 \mathrm{~h}^{-1}$ in sediment with corresponding $\mathrm{t}_{1 / 2}=7.4 \mathrm{~h}$ for copepods Coullana sp. in 24-h experiments (Lotufo 1998)

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=2.02-20.2 \mathrm{~h}$, based on estimated sunlight photolysis half-life in water (Howard et al. 1991); calculated atmospheric lifetime of 26 h based on gas-phase OH reactions (Brubaker \& Hites 1998).
Surface water: computed near-surface $\mathrm{t}_{1 / 2}=21 \mathrm{~h}$ for photochemical transformation of a water body (latitude $40^{\circ} \mathrm{N}$, midday, midsummer), $\mathrm{t}_{1 / 2}=160 \mathrm{~d}$ for direct photolysis in a $5-\mathrm{m}$ deep inland water body with no sedimentwater partitioning and $\mathrm{t}_{1 / 2}=200 \mathrm{~d}$ with sediment-water partitioning (Zepp \& Schlotzhauer 1979); $\mathrm{t}_{1 / 2}=21-63 \mathrm{~h}$, based on photolysis half-life in water (Howard et al. 1991); $\mathrm{t}_{1 / 2}=160 \mathrm{~d}$ for summer sunlight at $40^{\circ} \mathrm{N}$ latitude (Mill \& Mabey 1985).
Groundwater: $\mathrm{t}_{1 / 2}=6720-21120 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: desorption $\mathrm{t}_{1 / 2}=8.3 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $t_{1 / 2}=44-182$ d (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$\mathrm{t}_{1 / 2}=39 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and 34 d for $50 \mathrm{mg} / \mathrm{kg}$ treatment (Bulman et al. 1987);
biodegradation rate constant $\mathrm{k}=0.0018 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=377 \mathrm{~d}$ for Kidman sandy loam soil, and $\mathrm{k}=0.0026$ $\mathrm{d}^{-1}$ with $\mathrm{t}_{\mathrm{t} / 2}=268 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$\mathrm{t}_{1 / 2}=3360-10560 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
$\mathrm{t}_{1 / 2}=17.961 \mathrm{wk}, 7.8 \mathrm{yr}$ (Luddington soil, Wild et al. 1991).
Biota: $t_{1 / 2}=5$ d depuration half life by oysters (Lee et al. 1978);
elimination $\mathrm{t}_{1 / 2}=6 \mathrm{~d}$ from rainbow trout, $\mathrm{t}_{1 / 2}=2.0-29.8 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=8.4 \mathrm{~d}$ from clam Mya arenaria, $\mathrm{t}_{1 / 2}=5.8 \mathrm{~d}$ from polychaete Abarenicola pacifica, $\mathrm{t}_{1 / 2}=5.9 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=0.8 \mathrm{~d}$ from shrimp (Meador et al. 1995)
depuration $\mathrm{t}_{1 / 2} \sim 4.8 \mathrm{~h}$ in sediment and water for copepod $S$. knabeni, $\mathrm{t}_{1 / 2}=4.2 \mathrm{~h}$ in sediment and $\mathrm{t}_{1 / 2}=7.4 \mathrm{~h}$ in water for copepod Coullana sp. (Lotufo 1998)

TABLE 4.1.1.30.1
Reported aqueous solubilities of fluoranthene at various temperatures and reported temperature dependence equation

$$
\begin{equation*}
\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d} \tag{1}
\end{equation*}
$$

| May 1980, 1983 | May et al. 1978b |
| :---: | :---: |
| generator column-HPLC | generator column-HPLC/fluo. |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{\mathbf{- 3}}$ |
| 8.1 | 250.206 |
| 13.2 0.107 | $29 \quad 0.264$ |
| 19.7 0.1483 |  |
| 24.6 0.2027 | temp dependence eq. 1 |
| 29.9 | S $\quad \mu \mathrm{g} / \mathrm{kg}$ |
|  | a 0.0072 |
| temp dependence eq. 1 | b $\quad-0.1047$ |
| given in May et al. 1980 | c 4.322 |
| S $\quad \mu \mathrm{g} / \mathrm{kg}$ | d 50.4 |
| a 0.0072 |  |
| b $\quad-0.1047$ | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=39.83$ |
| c 4.322 | measured between 5-30 ${ }^{\circ} \mathrm{C}$ |
| d 50.4 |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=39.83 \\ & \text { measured between } 5-30^{\circ} \mathrm{C} \end{aligned}$ |  |



FIGURE 4.1.1.30.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for fluoranthene.

TABLE 4.1.1.30.2
Reported vapor pressures of fluoranthene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
(3)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| Tsypkina 1955 |  | Hoyer \& Peperle 1958 | Sonnefeld et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | effusion | generator column-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| 197.0 | 653 | data presented in eq. | 10.88 | $2.17 \times 10^{-4}$ |
| 209.0 | 1053 | eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | 10.88 | $2.05 \times 10^{-4}$ |
| 228.5 | 2586 | A 12.67 | 10.88 | $2.15 \times 10^{-4}$ |
| 238.1 | 3786 | B 5357 | 10.88 | $2.57 \times 10^{-4}$ |
| 247.7 | 5386 | for temp range $25-85^{\circ} \mathrm{C}$ | 20.25 | $7.07 \times 10^{-4}$ |
| 255.0 | 6586 |  | 20.25 | $7.39 \times 10^{-4}$ |
| 261.3 | 7919 | $\Delta \mathrm{H}_{\text {sub }}(\mathrm{kJ} / \mathrm{mol})=100$ | 20.25 | $7.25 \times 10^{-4}$ |
| 270.9 | 10319 |  | 20.25 | $7.63 \times 10^{-4}$ |
| 281.5 | 13386 |  | 29.79 | $2.03 \times 10^{-3}$ |
| 305.0 | 20318 |  | 29.79 | $1.99 \times 10^{-3}$ |
| 314.5 | 27384 |  | 29.80 | $2.17 \times 10^{-3}$ |
| 382.9 | 99058 |  | 29.80 | $2.20 \times 10^{-3}$ |
| 384.2 | 101325 |  | 38.9 | $5.81 \times 10^{-3}$ |
|  |  |  | 38.9 | $5.67 \times 10^{-3}$ |
|  |  |  | 38.9 | $5.58 \times 10^{-3}$ |
|  |  |  | 38.9 | $5.77 \times 10^{-3}$ |
|  |  |  | 38.9 | $5.46 \times 10^{-3}$ |
|  |  |  | 38.9 | $5.45 \times 10^{-3}$ |
|  |  |  | 25.0 | $1.23 \times 10^{-3}$ |
|  |  |  | eq. 2 | $\mathrm{P} / \mathrm{Pa}$ |
|  |  |  | A | 11.901 |
|  |  |  | B | 4415.56 |
|  |  |  | temp | $0-50^{\circ} \mathrm{C}$ |

[^3]

FIGURE 4.1.1.30.2 Logarithm of vapor pressure versus reciprocal temperature for fluoranthene.

TABLE 4.1.1.30.3
Reported Henry's law constants and octanol-air partition coefficients of fluoranthene at various temperatures and temperature dependence equations

| Henry's law constant |  |  |  | $\frac{\log \mathrm{K}_{\mathrm{OA}}}{\text { Harner \& Bidleman } 1998}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ten Hulscher et al. 1992 | Bamford et al. 1999 |  |  |  |  |
| gas stripping-HPLC/fluo. | gas stripping-GC/MS |  |  | generator column-GC/FID |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)$ | t/ ${ }^{\circ} \mathrm{C}$ | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | H/(Pa m ${ }^{3} / \mathrm{mol}$ ) | t/ ${ }^{\circ} \mathrm{C}$ | $\log \mathrm{K}_{\mathrm{OA}}$ |
|  |  |  | average |  |  |
| $10.0 \quad 0.26$ | 4.1 | 0.37. 0.49 | 0.56 | 0 | - |
| 20.0 0.64 | 11.0 | 0.79, 0.95 | 0.87 | 10 | - |
| $35.0 \quad 1.63$ | 18.0 | 1.21, 1.43 | 1.32 | 20 | 11.124 |
| 40.1 2.38 | 25.0 | 1.76, 2.18 | 1.96 | 30 | 8.652 |
| 45.0 5.84 | 31.0 | 2.36, 3.14 | 2.72 | 40 | 8.161 |
| $55.0 \quad 6.23$ |  |  |  | 25(exptl) | 8.88 |
|  |  |  |  | 25(calc) | 8.60 |
| $\ln \mathrm{K}_{\mathrm{AW}}=-\Delta \mathrm{H} / \mathrm{RT}+\Delta \mathrm{S} / \mathrm{R}$ | $\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  |  |  |
| $\mathrm{R}=8.314 \mathrm{~Pa} \mathrm{~m}^{3} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}$ | A | 8.4195 |  | $\log \mathrm{K}_{\mathrm{OA}}=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| $\Delta \mathrm{S} / \mathrm{R}$ | B | 4654.8 |  | A | -5.94 |
| $\Delta H / R \quad 6855.9$ |  |  |  | B | 4417 |
|  | enthalpy, entropy change: |  |  |  |  |
| enthalpy of volatilization: | $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{~mol}^{-1}\right)=38.7 \pm 2.5$ |  |  | enthalpy of phase change |  |
| $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{~mol}^{-1}\right)=57 \pm 5$ | $\Delta \mathrm{S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=70$ |  |  | $\Delta \mathrm{H}_{\mathrm{OA}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=$ |  |
| entropy of volatilization, $\Delta \mathrm{S}$ $\mathrm{T} \Delta \mathrm{S} /\left(\mathrm{kJ} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=54 \pm 5$ <br> at $20^{\circ} \mathrm{C}$ |  |  |  |  |  |



FIGURE 4.1.1.30.3 Logarithm of Henry's law constant and $K_{O A}$ versus reciprocal temperature for fluoranthene.

### 4.1.1.31 Benzo[a]fluorene



Common Name: Benzo[a]fluorene
Synonym: 1,2-benzofluorene, 11 H -benzo[ $a$ ]fluorene, chrysofluorene
Chemical Name: benzo[a]fluorene, 1,2-benzofluorene
CAS Registry No: 238-84-6
Molecular Formula: $\mathrm{C}_{17} \mathrm{H}_{12}$
Molecular Weight: 216.227
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
189.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ : 405 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
200.9 (Ruelle \& Kesselring 1997)
239.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
3.8, 18.4; 22.2 ( $126.75,189.65^{\circ} \mathrm{C}$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
39.76 (exptl., Chickos et al. 1999)
49.26, 50.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0243 ( mp at $189.5^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
0.045 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.045 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equation):
0.00136 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4373 /(\mathrm{T} / \mathrm{K})+11.80 ; \Delta \mathrm{H}_{\text {vap }}=-83.7 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated):
2.70* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-4113.54 /(\mathrm{T} / \mathrm{K})+6.976, \Delta \mathrm{H}=34.2 \mathrm{~kJ} \mathrm{~mol}^{-1}$, measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
5.68 (HPLC-RT correlation, Wang et al. 1986)
5.40 (recommended, Sangster 1989, 1993)
6.5387 (calculated-UNIFAC group contribution, Chen et al. 1993)
5.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k, or Half-Lives, $\mathrm{t}_{1 / 2}$ :

Half-Lives in the Environment:
Biota: elimination $\mathrm{t}_{1 / 2}=10.5 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=4.2 \mathrm{~d}$ from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.31.1
Reported Henry's law constants of benzo[a]fluorene at various temperatures
Bamford et al. 1999

| gas stripping-GC/MS |  |  |
| :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ |
|  | average |  |
| 4.1 | $0.67,1.16$ | 0.88 |
| 11.0 | $1.08,1.57$ | 1.30 |
| 18.0 | $1.61 ., 2.23$ | 1.89 |
| 25.0 | $2.19,3.33$ | 2.70 |
| 31.0 | $2.74,4.78$ | 3.62 |
| $\ln \mathrm{~K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |  |
| A | 6.9762 |  |
| B | 4113.5 |  |
| enthalpy, entropy change: |  |  |
| $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=34.2 \pm 4.9$ |  |  |
| $\Delta \mathrm{~S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=58$ |  |  |

at $25^{\circ} \mathrm{C}$


FIGURE 4.1.1.31.1 Logarithm of Henry's law constant versus reciprocal temperature for benzo[a]fluorene.

### 4.1.1.32 Benzo[b]fluorene



Common Name: Benzo[b]fluorene
Synonym: 2,3-benzofluorene, 11H-benzo[b]fluorene, isonaphthofluorene
Chemical Name: benzo[b]fluorene
CAS Registry No: 243-17-4
Molecular Formula: $\mathrm{C}_{17} \mathrm{H}_{12}$
Molecular Weight: 216.227
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
212 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
401 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
200.9 (Ruelle \& Kesselring 1997)
239.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
23.4 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 47.78, 50.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.0146\left(\mathrm{mp}\right.$ at $212^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0020 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.002 (average lit. value, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$7.37 \times 10^{-6 *}$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $71-125^{\circ} \mathrm{C}, \mathrm{Oja}$ \& Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=36.325-14354 /(\mathrm{T} / \mathrm{K})$; temp range $344-398 \mathrm{~K}$ (Antoine eq., Knudsen effusion, Oja \& Suuberg 1998) 0.00107 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4423 /(\mathrm{T} / \mathrm{K})+11.86 ; \Delta \mathrm{H}_{\text {vap }} .=-84.7 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
5.77 (HPLC-RT correlation, Wang et al. 1986)
5.75 (recommended, Sangster 1989, 1994)
5.77 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :

Half-Lives in the Environment:
Biota: elimination $\mathrm{t}_{1 / 2}=10.5 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=4.3 \mathrm{~d}$ from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.32.1
Reported vapor pressures of benzo[b]fluorene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(2) $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

Oja \& Suuberg 1998

| Knudsen effusion |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 70.92 | 0.00454 |
| 83.14 | 0.0188 |
| 97.55 | 0.0936 |
| 124.4 | 1.230 |
|  |  |
| $\mathrm{mp} / \mathrm{K}$ | $484-486$ |
|  |  |
| eq. 1a |  |
| A | $\mathrm{P} / \mathrm{Pa}$ |
| B | 36.325 |
| for temp range $344-398 \mathrm{~K}$ |  |
| $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ} / \mathrm{mol})=119.3$ |  |



FIGURE 4.1.1.32.1 Logarithm of vapor pressure versus reciprocal temperature for benzo[b]fluorene.

### 4.1.1.33 Chrysene



Common Name: Chrysene
Synonym: 1,2-benzophenanthrene, benzo( $a$ )phenanthrene, 1,2,5,6-dibenzonaphthalene
Chemical Name: chrysene
CAS Registry No: 218-01-9
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{12}$
Molecular Weight: 228.288
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
255.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
448 (Weast 1975; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.274 (Weast 1982-83; Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$179.2\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
250.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }} \mathrm{cal} / \mathrm{mol}$ :
26.153 (Ruelle \& Kesselring 1997)
3.22, 26.15; 29.37 ( $239.05,28.25^{\circ} \mathrm{C}$, total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
49.37 (Casellato et al. 1973)
62.34 (Ubbelohde 1978)
49.21 (Chickos et al. 1999)
55.5, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.00548 ( mp at $255.5^{\circ} \mathrm{C}$ )
0.00976 (calculated, Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$0.0015 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.006 (shake flask-UV, Klevens 1950)
0.0015 (Weimer \& Prausnitz 1965)
0.0041, 0.0014 (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)
0.002 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.0018 (Rossi 1977; Neff 1979; quoted, Eadie et al. 1982)
0.0018* (generator column-HPLC/UV, measured range $6.5-29^{\circ} \mathrm{C}$ May et al. 1978a,b)
$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=0.609+0.0144 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+0.0024 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}$; temp range $5-30^{\circ} \mathrm{C}$ (generator column-HPLC/UV, May et al. 1978)
0.017 (shake flask-nephelometry, Hollifield 1979)
0.00189* $\quad\left(25.3^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range 279.65-301.85 K, May et al. 1983)
0.0018* (average lit. value, Pearlman et al. 1984)
0.00327 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
$0.00102,0.0012$ (generator column-HPLC/UV, Billington et al. 1988)
0.0019 (recommended, Shaw 1989)
0.0016 (generator column-HPLC, Vadas et al. 1991)
0.0015 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-0.323-1369 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$5.7 \times 10^{-7 *}$ (effusion method, extrapolated, De Kruif 1980)
$8.4 \times 10^{-7} \quad$ (effusion method, Hoyer \& Peperle 1958; quoted, Mabey et al. 1982)
$\log (\mathrm{P} / \mathrm{mmHg})=13.07-6340 /(\mathrm{T} / \mathrm{K})$; temp range $80-145^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958)
$6.08 \times 10^{-7}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.445-6160 /(\mathrm{T} / \mathrm{K})$; temp range $358-463 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-50.1566-3.4381 \times 10^{3} /(\mathrm{T} / \mathrm{K})+25.178 \cdot \log (\mathrm{~T} / \mathrm{K})-2.462 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+7.1044 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$ temp range 531-979 K (vapor pressure eq., Yaws 1994)
$2.29 \times 10^{-4}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, quoted, Finizio et al. 1997)
$5.70 \times 10^{-7} ; 5.84 \times 10^{-5}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with
fugacity ratio F , Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.24-5507 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.66-4139 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{Pa})=14.848-6189 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
$1.70 \times 10^{-4} \quad$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4679 /(\mathrm{T} / \mathrm{K})+11.92 ; \Delta \mathrm{H}_{\text {vap }} .=-89.6 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
$2.11 \times 10^{-6}$ (solid $\mathrm{P}_{\mathrm{S}}$, gas saturation-GC/MS, Mader \& Pankow 2003)
$4.03 \times 10^{-4}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from $\mathrm{P}_{\mathrm{S}}$ assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Mader \& Pankow 2003)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.107 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
0.53* (gas stripping-GC, measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-12136.2 /(\mathrm{T} / \mathrm{K})+32.235, \Delta \mathrm{H}=100.9 \mathrm{~kJ} \mathrm{~mol}^{-1}$, measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left(\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right)=9.98-2770 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
0.53 (quoted, Dachs \& Eisenreich 2000)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
5.79 (HPLC-k' correlation, Hanai et al. 1981)
5.91 (RP-TLC-k' correlation, Bruggeman et al. 1982)
5.73 (HPLC-RT correlation, Wang et al. 1986)
$5.61 \pm 0.40$ (recommended, Sangster 1989)
5.84 (TLC retention time correlation, De Voogt et al. 1990)
5.50 (shake flask-UV, Alcorn et al. 1993)
5.86 (recommended, Sangster 1993)
5.73 (recommended, Hansch et al. 1995)
5.81 (range 6.63-5.94) (shake flask/slow stirring-HPLC/fluo., De Maagd et al. 1998)
5.78 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson \& Schröader 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
10.40 (calculated- $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, Wania \& Mackay 1996)
10.44 (calculated, Finizio et al. 1997)

Bioconcentration Factor, $\log$ BCF:

| 4.31 | $(P$. hoyi, Eadie et al. 1982) |
| :--- | :--- |
| 4.72 | (microorganisms-water, calculated from $\mathrm{K}_{\mathrm{OW}}$, Mabey et al. 1982) |
| 3.785 | (Daphnia magna, Newsted \& Giesy 1987) |
| $1.17,0.792$ | (Polychaete sp, Capitella capitata, Bayona et al. 1991) |

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
6.27 (sediments average, Kayal \& Connell 1990)
6.9 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
4.0 (predicted dissolved $\log \mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)
5.79 (5.74-5.83), 5.40 (5.35-5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flaskHPLC/UV, de Maagd et al. 1998)
5.52-7.38; 4.90-7.80 (for chrysene + triphenylene, range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
5.92; 6.12, 5.77, 6.14 (for chrysene + triphenylene, $20^{\circ} \mathrm{C}$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt $1,2,3$-solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: calculated $\mathrm{t}_{1 / 2}=4.4 \mathrm{~h}$ of direct sunlight photolysis for $50 \%$ conversion at $40^{\circ} \mathrm{N}$ latitude of midday in midsummer: 4.4 h in near-surface water; (Herbes et al. 1980)
direct photochemical transformation $\mathrm{t}_{1 / 2}($ calc $)=4.4 \mathrm{~h}$, computed near-surface water, latitude $40^{\circ} \mathrm{N}$, midday, midsummer and photolysis $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ and 68 d in $5-\mathrm{m}$ deep inland water body without and with sedimentwater partitioning, respectively, to top cm of bottom sediment over full summer day, $40^{\circ} \mathrm{N}$ (Zepp \& Schlotzhauer 1979)
$\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ in $5-\mathrm{m}$ deep inland water and $\mathrm{t}_{1 / 2}=68 \mathrm{~d}$ in inland water with sediment partitioning (Zepp \& Schlotzhauer 1979)
half-lives on different atmospheric particulate substrates (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=100 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=78 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=38 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985)
first order daytime decay constants:: $\mathrm{k}=0.0056 \mathrm{~min}^{-1}$ for soot particles loading of $1000-2000 \mathrm{ng} / \mathrm{mg}$ and $\mathrm{k}=0.0090 \mathrm{~min}^{-1}$ with $30-350 \mathrm{ng} / \mathrm{mg}$ loading (Kamens et al. 1988)
photodegradation $\mathrm{k}=7.07 \times 10^{-3} \mathrm{~min}$ with $\mathrm{t}_{1 / 2}=1.63 \mathrm{~h}$ in ethanol-water ( $1: 1, \mathrm{v} / \mathrm{v}$ ) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
$\mathrm{k}($ exptl $)=0.00707 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=1.63 \mathrm{~h}$ and the predicted $\mathrm{k}=0.0114 \mathrm{~min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
$\mathrm{k}=1.01-1.30 \mathrm{~min}^{-1}$ in natural water system by UV and sunlight (Yu et al. 1999)
$\mathrm{t}_{1 / 2}(\mathrm{obs})=1.58 \mathrm{~h}, \mathrm{t}_{1 / 2}($ calc $)=1.34 \mathrm{~h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
photochemical degradation $\mathrm{k}=(1.60 \pm 0.08) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(11.99 \pm 0.53) \mathrm{h}$ in diesel particulate matter under atmospheric conditions; $\mathrm{k}=(2.29 \pm 0.22) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(8.41 \pm 0.91) \mathrm{h}$ in diesel particulate matter/soil mixture, and $\mathrm{t}_{1 / 2}=1.69-8.82 \mathrm{~h}$ in various soil components using a $900-\mathrm{W}$ photo-irradiator as light source; $\mathrm{k}=(4.76 \pm 0.40) \times 10^{-7} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(405.26 \pm 37.27) \mathrm{h}$ in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)
Photodegradation $\mathrm{k}=9.0 \times 10^{-5} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: $t_{1 / 2}=2.6 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
$\mathrm{k}>1 \times 10^{6} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=1 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982);
photooxidation $\mathrm{t}_{1 / 2}=0.802-8.02 \mathrm{~h}$ in air, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991)
Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation: significant degradation with gradual adaptation within 7 d for a domestic sewer 28 d test for an average of three static-flask screening (Tabak et al. 1981)
aerobic $\mathrm{t}_{1 / 2}=8904-24000 \mathrm{~h}$, based on aerobic soil dieaway test data (Howard et al. 1991)
rate constants $\mathrm{k}=0.0019 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=371 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0018 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=387 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
anaerobic $\mathrm{t}_{1 / 2}=35616-96000 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation: estimated to be $1 \times 10^{-10} \mathrm{~mL}^{\text {cell }}{ }^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=0.35-0.71 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.15 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.802-8.02 \mathrm{~h}$, based on estimated photooxidation half-life in air (Howard et al. 1987);
$t_{1 / 2}=1.3 \mathrm{~h}$ for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated rate constant $\mathrm{k}=0.0092 \mathrm{~min}^{-1}$ at $1 \mathrm{cal} \mathrm{cm}^{-2} \mathrm{~min}^{-1}, 10 \mathrm{~g} / \mathrm{m}^{3} \mathrm{H}_{2} \mathrm{O}$ and $20^{\circ} \mathrm{C}$ (Kamens et al. 1988).
Surface water: photolysis $\mathrm{t}_{1 / 2}=4.4 \mathrm{~h}$ near surface water, $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ and 68 d in $5-\mathrm{m}$ deep water body without and with sediment-water partitioning in full summer day, $40^{\circ} \mathrm{N}$; photosensitized oxygenation $\mathrm{t}_{1 / 2}=2.6 \mathrm{~h}$ at near surface water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
$\mathrm{t}_{1 / 2} \sim 4.4-13 \mathrm{~h}$, based on photolysis half-life in water (Howard et al. 1991);
photolysis $t_{1 / 2}=1.63 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996);
photolysis $\mathrm{t}_{1 / 2}=533-693 \mathrm{~min}$ at $18^{\circ} \mathrm{C}$ in natural water system by UV and sunlight illumination (Yu et al. 1999).
Groundwater: $t_{1 / 2}=17808-48000 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: desorption $t_{1 / 2}=31.9 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $\mathrm{t}_{1 / 2} .>5.5 \mathrm{~d}$ (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$t_{1 / 2}=328 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and $\mathrm{t}_{1 / 2}=224 \mathrm{~d}$ for $50 \mathrm{mg} / \mathrm{kg}$ treatment (Bulman et al. 1987);
biodegradation rate constant $1=0.0019 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=371 \mathrm{~d}$ for Kidman sandy loam soil, and $\mathrm{k}=0.0018$ $\mathrm{h}^{-1}$ with $\mathrm{t}_{1 / 2}=387 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$t_{1 / 2}=8904-24000 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991);
$t_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988).
Biota: elimination $\mathrm{t}_{1 / 2}=5.0-14.2 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=15.1 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=4.3 \mathrm{~d}$ from clam Mercenario mercenaria, $\mathrm{t}_{1 / 2}=3.3 \mathrm{~d}$ from clam Macoma balthica (quoted, Meador et al. 1995).

TABLE 4.1.1.33.1
Reported aqueous solubilities of chrysene at various temperatures and reported temperature dependence equations

$$
\begin{equation*}
S /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d} \tag{1}
\end{equation*}
$$




FIGURE 4.1.1.33.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for chrysene.

TABLE 4.1.1.33.2
Reported vapor pressures and Henry's law constants of chrysene at various temperatures and temperature dependence equations



FIGURE 4.1.1.33.2 Logarithm of vapor pressure and Henry's law constant versus reciprocal temperature for chrysene.

### 4.1.1.34 Triphenylene



Common Name: Triphenylene
Synonym: 9,10-benzophenanthrene, isochrysene, 1,2,3,4-dibenznaphthalene
Chemical Name: triphenylene
CAS Registry No: 217-59-4
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{12}$
Molecular Weight: 228.288
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
197.8 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
425 (Weast 1982-83; Dean 1985; Pearlman et al. 1984; Budavari 1989; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
1.302 (Dean 1985; Budavari 1989)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
211.8 (Ruelle \& Kesselring 1997)
250.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
24.74 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
52.53, 44.1 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0202\left(\mathrm{mp}\right.$ at $197.8^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.0388 \quad\left(27^{\circ} \mathrm{C}\right.$, nephelometry, Davis et al. 1942)
0.043 (shake flask-UV, Klevens 1950)
0.043 (shake flask-fluorescence, Mackay \& Shiu 1977)
$0.0049^{*} \quad\left(20.5^{\circ} \mathrm{C}\right.$, generator column-HPLC, measured range 281.15-301.35 K, May et al. 1983)
0.041 (lit. mean, Pearlman et al. 1984)
0.0307 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
0.041 (vapor saturation-UV, Akiyoshi et al. 1987)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$\log (\mathrm{P} / \mathrm{mmHg})=12.89-6154 /(\mathrm{T} / \mathrm{K})$; temp range: $65-125^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958) $2.30 \times 10^{-6 *}$ (effusion, De Kruif 1980)
$3.85 \times 10^{-7}$ (extrapolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=9.435-5620 /(\mathrm{T} / \mathrm{K})$; temp range: $363-468 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$1.17 \times 10^{-2}$ (extrapolated-Antoine eq.-II, supercooled liquid $\mathrm{P}_{\mathrm{L}}$, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.8974-3527 /(\mathrm{T} / \mathrm{K})$; temp range: $600-720 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987) $2.39 \times 10^{-4}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4624 /(\mathrm{T} / \mathrm{K})+11.89 ; \Delta \mathrm{H}_{\text {vap }} .=-88.5 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations:
5.45 (shake flask-UV, Karickhoff et al. 1979)
5.49 (HPLC-RT correlation, Wang et al. 1986)
(TLC retention time correlation, De Voogt et al. 1990)
5.49 (recommended, Sangster 1993)
5.49 (recommended, Hansch et al. 1995)
5.15; 4.83 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)
$\log \mathrm{K}_{\text {ow }}=1.313+1138.55 /(\mathrm{T} / \mathrm{K})$; temp range $5-55^{\circ} \mathrm{C}$ (temperature dependence HPLC-k' correlation, Lei et al. 2000)
6.27 (RP-HPLC-RT correlation, short ODP column, Donovan \& Pescatore 2002)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
3.96 (Daphnia magna, Newsted \& Giesy 1987)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
6.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
4.0 (predicted dissolved $\log \mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)
5.52-7.38; 4.90-7.80 (for chrysene + triphenylene, range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
5.92; 6.12, 5.77, 6.14 (for chrysene + triphenylene, $20^{\circ} \mathrm{C}$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt $1,2,3$-solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Biota: elimination $t_{1 / 2}=2 \mathrm{~d}$ from rainbow trout, $\mathrm{t}_{1 / 2}=4.4 \mathrm{~d}$ from clam Mya arenaria, $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$ from mussel Mytilus edulis, $\mathrm{t}_{1 / 2}=14.4 \mathrm{~d}$ from polychaete Abarenicola pacifica, $\mathrm{t}_{1 / 2}=21.7 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=2.4 \mathrm{~d}$ from shrimp (quoted, Meador et al. 1995).

## TABLE 4.1.1.34.1

Reported aqueous solubilities and vapor pressures of triphenylene at various temperatures and reported temperature dependence equation

$$
\begin{equation*}
\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d} \tag{1}
\end{equation*}
$$

Aqueous solubility

| May 1980, May et al. 1983 |  | Hoye | 1958 |
| :---: | :---: | :---: | :---: |
| generator column-HPLC |  | effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 8.0 | 0.00299 | da |  |
| 12.0 | 0.00393 | $\log \mathrm{P} /$ | 3/(T/K) |
| 14.8 | 0.00339 | A | 12.89 |
| 20.5 | 0.00489 | B | 6154 |
| 27.3 | 0.00765 | temp | $5^{\circ} \mathrm{C}$ |
| 28.2 | 0.00811 |  |  |
| temp dependence eq. 1 given in May 1980 |  |  |  |
| S | $\mu \mathrm{g} / \mathrm{kg}$ |  |  |
| a | -0.0002 |  |  |
| b | 0.0250 |  |  |
| c | -0.4250 |  |  |
| d | 4.89 |  |  |
| $\begin{aligned} & \Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=41.25 \\ & \text { measured between } 5-30^{\circ} \mathrm{C} \end{aligned}$ |  |  |  |

measured between $5-30^{\circ} \mathrm{C}$

Vapor pressure

| Vapor pressure |  |
| :---: | :---: |
| Hoyer \& Peperle 1958 | de Kruif 1980 |
| effusion | torsion, weighing effusion |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ |
| data presented by | 107.02 0.1 |
| $\log \mathrm{P} / \mathrm{mmHg}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | 114.36 0.2 |
| A 12.89 | 118.39 0.3 |
| B 6154 | 134.52 0.4 |
| temp range $65-125^{\circ} \mathrm{C}$ | 122.0 0.5 |
|  | 126.61 0.6 |
| $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=114.6$ | 128.38 0.7 |
|  | 129.94 0.8 |
|  | 131.32 0.9 |
|  | 132.56 1.0 |
|  | $\begin{array}{cc} 25.0 & \begin{array}{c} 2.3 \times 10^{-6} \\ \text { extrapolated } \end{array} \end{array}$ |
|  | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=115.2$ |



FIGURE 4.1.1.34.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for triphenylene.

### 4.1.1.35 o-Terphenyl



Common Name: o-Terphenyl
Synonym: 1,2-diphenyl benzene
Chemical Name:
CAS Registry No: 84-15-1
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{14}, 1,2-\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{2} \mathrm{C}_{6} \mathrm{H}_{4}$
Molecular Weight: 230.304
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
56.2 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
332 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$225.4 \quad\left(93^{\circ} \mathrm{C}\right.$, Stephenson \& Malanowski 1987)
273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
17.2 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
52.3, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.494 ( mp at $56.2^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
1.24 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{kPa})=6.29308-[2160.24 /(-106.38+(\mathrm{T} / \mathrm{K})]$; temp range $462-650 \mathrm{~K}$ (Antoine eq., liquid phase, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-8.0641-4.0928 \times 10^{3} /(\mathrm{T} / \mathrm{K})+9.1076 \cdot \log (\mathrm{~T} / \mathrm{K})-1.6326 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+6.0467 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range 329-891 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Air:
Surface water: a first order reduction process in river water with an estimated $t_{1 / 2}=0.6 \mathrm{~d}$ for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).
Ground water:
Sediment:
Soil:
Biota:

### 4.1.1.36 $m$-Terphenyl



Common Name: $m$-Terphenyl
Synonym: 1,3-diphenyl benzene
Chemical Name:
CAS Registry No: 92-06-8
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{14}, 1,3-\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{2} \mathrm{C}_{6} \mathrm{H}_{4}$
Molecular Weight: 230.304
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
87 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
363 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.199 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$227 \quad\left(93^{\circ} \mathrm{C}\right.$, Stephenson \& Malanowski 1987)
$192.1 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
22.59 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 62.76, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.246 (mp at $87^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1.51 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)
$0.0305^{*} \quad\left(24.99^{\circ} \mathrm{C}\right.$, generator column-HPLC/fluorescence, Reza et al. 2002)
$\ln x=(-2.62 \pm 0.91)+(-5134 \pm 271) /(\mathrm{T} / \mathrm{K})$; temp range 278-323.13 K (Reza et al. 2002)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$\log (\mathrm{P} / \mathrm{kPa})=6.48808-[2445.98 /(-102.76+(\mathrm{T} / \mathrm{K})]$; temp range $462-691 \mathrm{~K}$ (Antoine eq., liquid phase, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-14.7175-4.3577 \times 10^{3} /(\mathrm{T} / \mathrm{K})+11.935 \cdot \log (\mathrm{~T} / \mathrm{K})-1.8441 \times 10^{-2} \cdot(\mathrm{~T} / \mathrm{K})+6.437 \times 10^{-6} \cdot(\mathrm{~T} / \mathrm{K})^{2} ;$ temp range $360-925 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Air:
Surface water: a first order reduction process in river water with an estimated $t_{1 / 2}=0.6 \mathrm{~d}$ for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

Ground water:
Sediment:
Soil:
Biota:

TABLE 4.1.1.36.1
Reported aqueous solubilities of m-terphenyl at various temperatures

Reza et al. 2002

| generator column-HPLC |  |  |  |
| :---: | :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 4.85 | 0.009 | 40.07 | 0.0741 |
| 7.64 | 0.0115 | 45.07 | 0.095 |
| 11.8 | 0.012 | 49.98 | 0.1159 |
| 14.98 | 0.0183 | $\ln x=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| 19.95 | 0.0219 | A | -2.62 |
| 24.99 | 0.0305 | B | 5134 |
| 30.0 | 0.0409 | for temp range $287-323 \mathrm{~K}$ |  |
| 35.0 | 0.0535 |  |  |



FIGURE 4.1.1.36.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for $m$-terphenyl.

### 4.1.1.37 $p$-Terphenyl



Common Name: $p$-Terphenyl
Synonym: 1,4-diphenyl benzene
Chemical Name: $p$-terphenyl
CAS Registry No: 92-94-4
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{14}, 1,4-\left(\mathrm{C}_{6} \mathrm{H}_{5}\right)_{2} \mathrm{C}_{6} \mathrm{H}_{4}$
Molecular Weight: 230.304
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
213.9 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
376 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$262.0 \quad\left(315.6^{\circ} \mathrm{C}\right.$, Stephenson \& Malanowski 1987)
273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
$0.3,35.3 ; 35.6 \quad\left(-79.55,213.85^{\circ} \mathrm{C}\right.$; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
74.1, 73.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.014 (mp at $213.9^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
1.80 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$4.86 \times 10^{-6}$ (extrapolated from solid, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.515-6210 /(\mathrm{T} / \mathrm{K})$; temp range $338-431 \mathrm{~K}$ (Antoine eq.-I, solid phase, Stephenson \& Malanowski 1987)
$1.78 \times 10^{-5} \quad\left(\mathrm{P}_{\mathrm{L}}\right.$ extrapolated from liquid state, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.16107-[2125.84 /(-145.29+(\mathrm{T} / \mathrm{K})]$; temp range $499-700 \mathrm{~K}$ (Antoine eq.-II, liquid phase, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{mmHg})=-39.6342-3.2661 \times 10^{3} /(\mathrm{T} / \mathrm{K})+21.08 \cdot \log (\mathrm{~T} / \mathrm{K})-2.2574 \times 10^{-2} .(\mathrm{T} / \mathrm{K})+6.902 \times 10^{-6} .(\mathrm{T} / \mathrm{K})^{2} ;$
temp range $485-926 \mathrm{~K}$ (vapor pressure eq., Yaws 1994)
$5.40 \times 10^{-4}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4135 /(\mathrm{T} / \mathrm{K})+10.60 ; \Delta \mathrm{H}_{\text {vap }}=-79.2 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
6.03, 5.88 (HPLC-RV correlation, Garst 1984) $6.03 \pm 0.50$ (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :

Half-Lives in the Environment:
Air:
Surface water: a first order reduction process in river water with an estimated $t_{1 / 2}=0.6 \mathrm{~d}$ for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).
Ground water:
Sediment:
Soil:
Biota:

### 4.1.1.38 Naphthacene



Common Name: Naphthacene
Synonym: benz[ $b]$ anthracene, 2,3-benzanthracene, tetracene
Chemical Name: benz[ $b$ ]anthracene
CAS Registry No: 92-24-0
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{12}$
Molecular Weight: 228.288
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
357 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
450 (sublimation, Bjørseth 1983; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
211.8 (Ruelle \& Kesselring 1997)
250.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
38.64 (Ruelle \& Kesselring 1997)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.000553\left(\mathrm{mp}\right.$ at $\left.357^{\circ} \mathrm{C}\right)$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$0.0010 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.0015 (approximate, shake flask-UV, Klevens 1950)
0.0036 (shake flask-UV, Eisenbrand \& Baumann 1970)
0.00057 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.044 (shake flask-nephelometry, Hollifield 1979)
0.00103 (lit. mean, Pearlman et al. 1984)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$7.30 \times 10^{-9 *} \quad$ (effusion method, De Kruif 1980)
$3.70 \times 10^{-8} \quad$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.505-6540 /(\mathrm{T} / \mathrm{K})$; temp range $376-489 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$2.31 \times 10^{-8 *} \quad$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $113-199^{\circ} \mathrm{C}$,
Oja \& Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=33.594-15151 /(\mathrm{T} / \mathrm{K})$; temp range $368-472 \mathrm{~K}$ (Antoine eq., Knudsen effusion, Oja \& Suuberg 1998)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
5.90 (shake flask-UV, concn. ratio, Karickhoff et al., 1979)
6.02 (HPLC-k' correlation, McDuffie 1981)
5.76 (HPLC-RT correlation, Wang et al. 1986)
5.76. (recommended, Sangster 1989, 1993)
5.84 (TLC retention time correlation, De Voogt et al. 1990)
5.90 (shake flask-HPLC, De Voogt et al. 1990)
5.90 (recommended, Hansch et al 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
5.81 (sediment, batch equilibrium-sorption isotherms by GC/UV, Karickhoff et al. 1979)

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis: direct photochemical transformation $\mathrm{t}_{1 / 2}=0.034 \mathrm{~h}$, computed near-surface water, latitude $40^{\circ} \mathrm{N}$, midday, midsummer and photolysis $\mathrm{t}_{1 / 2}=0.20 \mathrm{~d}$ and 0.95 d in $5-\mathrm{m}$ deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, $40^{\circ} \mathrm{N}$ (Zepp \& Schlotzhauer 1979)
photodegradation $\mathrm{k}=0.051 \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=0.23 \mathrm{~h}$ in ethanol-water ( $1: 1, \mathrm{v} / \mathrm{v}$ ) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
pseudo-first-order direct photolysis $\mathrm{k}($ exptl $)=0.051 \mathrm{~min}^{-1}$ with the calculated $\mathrm{k}=0.051 \mathrm{~min}^{-1}$ and $\mathrm{t} / 1 / 2=0.23$ h and the predicted $\mathrm{k}($ calc $)=0.0355 \mathrm{~min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996) direct photolysis $\mathrm{t}_{1 / 2}=0.92 \mathrm{~h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001).
Oxidation: $\mathrm{t}_{1 / 2}=2.6 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: direct photolysis $t_{1 / 2}=0.92 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).
Surface water: photolysis $\mathrm{t}_{1 / 2}=0.034 \mathrm{~h}$ near surface water, $\mathrm{t}_{1 / 2}=0.20 \mathrm{~d}$ and 0.95 d in $5-\mathrm{m}$ deep water body without and with sediment-water partitioning in full summer day, $40^{\circ} \mathrm{N}$; photosensitized oxygenation $\mathrm{t}_{1 / 2}=2.6 \mathrm{~h}$ at near surface water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979).
photolysis $\mathrm{t}_{1 / 2}=0.23 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

## TABLE 4.1.1.38.1

Reported vapor pressures of naphthacene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
de Kruif $1980 \quad$ Oja \& Suuberg 1998

| torsion-, weighing effusion |  |  | Knudsen effusion |  |
| :--- | :---: | :--- | :--- | :--- |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |  | $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 147.35 | 0.1 |  | 113.4 | 0.00344 |
| 155.46 | 0.2 |  | 128.78 | 0.0199 |
| 160.35 | 0.3 |  | 139.56 | 0.0535 |
| 163.89 | 0.4 |  | 145.44 | 0.0496 |
| 166.67 | 0.5 |  | 160.69 | 0.322 |
| 168.97 | 0.6 |  | 172.88 | 0.584 |
| 170.94 | 0.7 |  | 198.99 | 4.81 |
| 172.65 | 0.8 |  |  |  |
| 173.98 | 0.9 |  | $\mathrm{mp} / \mathrm{K}$ | 630 |
| 175.65 | 1.0 |  |  |  |

TABLE 4.1.1.38.1 (Continued)

| de Kruif 1980 | Oja \& Suuberg 1998 |
| :---: | :---: |
| torsion-, weighing effusion | Knudsen effusion |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ |
| $25.0 \quad$$9.7 \times 10^{-9}$ <br> extrapolated | eq. 1a $\mathrm{P} / \mathrm{Pa}$ <br> A 35.594 |
| $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=155.0$ | for temp range 386-472 K $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=126.1$ |



FIGURE 4.1.1.38.1 Logarithm of vapor pressure versus reciprocal temperature for naphthacene.

### 4.1.1.39 Benz[a]anthracene



Common Name: Benz[ $a$ anthracene
Synonym: 1,2-benzanthracene, 2,3-benzophenanthrene, naphthanthracene, BaA, B(a) a, tetraphene
Chemical Name: 1,2-benzanthracene
CAS Registry No: 56-55-3
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{12}$
Molecular Weight: 228.288
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
160.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
438 (Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
1.2544 (Mailhot \& Peters 1988)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
211.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999) 248.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
21.38 (Ruelle \& Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 49.23, 44.1 (exptl., calculated-group additivity method, Chickos et al. 1999) 49.2 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), $\mathrm{F}: 0.0468$ ( mp at $160.5^{\circ} \mathrm{C}$ ) 0.040 (calculated, assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Mackay et al. 1980) 0.0661 (calculated, $\Delta \mathrm{S}_{\text {fus }}=49.2 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

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0.011 (27 C C, shake flask-nephelometry, Davis & Parker 1942)
0.010 (shake flask-UV, Klevens 1950)
0.014 (shake flask-fluorescence, Mackay & Shiu 1977)
0.0094, 0.0122 (25, 29 ' C, generator column-HPLC/UV, May et al. 1978b)
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$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=1.74+0.1897 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)+0.0031 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{2}+0.0003 \cdot\left(\mathrm{t} /{ }^{\circ} \mathrm{C}\right)^{3}$, temp range $5-30^{\circ} \mathrm{C}$ (generator column-
HPLC/UV, May et al. 1978b, May 1980)
0.044 (shake flask-nephelometry, Hollifield 1979)
0.00837* (generator column-HPLC, measured range 6.9-29.7${ }^{\circ} \mathrm{C}$, May 1980)
0.0086* (generator column-HPLC, measured range $6.9-29.7^{\circ} \mathrm{C}$, May et al. 1983)
0.00935* (generator column-fluo., measured range $10-30^{\circ} \mathrm{C}$, Velapoldi et al. 1983)
0.011 (average lit. value, Pearlman et al. 1984)
0.0168 (generator column-HPLC/fluorescence, Walters \& Luthy 1984)
0.00854 (generator column-HPLC/UV, measured range $3.7-25.0^{\circ} \mathrm{C}$, Whitehouse 1984)
0.011 (recommended, IUPAC Solubility Data Series, Shaw 1989)
0.0146 (shake flask-HPLC, Haines \& Sandler 1995)
0.0130 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-0.326-1119 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=-3.060466-5354.51 /(\mathrm{T} / \mathrm{K})$, temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section): $2.93 \times 10^{-6}\left(20^{\circ} \mathrm{C}\right.$, Hoyer \& Peperle 1958) $\log (\mathrm{P} / \mathrm{mmHg})=13.68-6250 /(\mathrm{T} / \mathrm{K})$; temp range $60-120^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958)
$2.17 \times 10^{-5}$ (solid, extrapolated from Antoine eq., Kelley \& Rice 1964; quoted, Bidleman 1984)
$\log (\mathrm{P} / \mathrm{mmHg})=11.528-5461 /(\mathrm{T} / \mathrm{K})$; temp range: $104-127^{\circ} \mathrm{C}$ (effusion method, Kelley \& Rice 1964)
$3.87 \times 10^{-7}$ (effusion method, Wakayama \& Inokuchi 1967)
$1.47 \times 10^{-5}$ (solid, effusion method, extrapolated-Antoine eq., Murray et al. 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=10.045-5929 /(\mathrm{T} / \mathrm{K})$; temp range: $330-390 \mathrm{~K}$ (effusion method, Murray et al. 1974)
$6.67 \times 10^{-7}\left(20^{\circ} \mathrm{C}\right.$, effusion, Pupp et al. 1974)
$7.30 \times 10^{-6 *}$ (effusion method, De Kruif 1980)
$2.71 \times 10^{-5 *}$ (gas saturation-HPLC/fluo./UV, Sonnefeld et al. 1983)
$\log (\mathrm{P} / \mathrm{Pa})=9.684-4246.51 /(\mathrm{T} / \mathrm{K})$; temp range $10-50^{\circ} \mathrm{C}$ (solid, Antoine eq., Sonnefeld et al. 1983)
$0.00107,0.0003$ ( $\mathrm{P}_{\mathrm{GC}}$ by GC-RT correlation, different GC columns, Bidleman 1984)
0.000543 (supercooled liquid $P_{L}$, converted from literature $P_{S}$ with $\Delta S_{\text {fus }}$ Bidleman 1984)
$2.49 \times 10^{-4}$ (Yamasaki et al. 1984)
$4.10 \times 10^{-6}$ (selected, Howard et al. 1986)
$1.51 \times 10^{-5}, 2.17 \times 10^{-5}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.0507-5925 /(\mathrm{T} / \mathrm{K})$; temp range $330-390 \mathrm{~K}$ (solid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.653-5461 /(\mathrm{T} / \mathrm{K})$; temp range $377-400 \mathrm{~K}$ (solid, Antoine eq-II., Stephenson \& Malanowski 1987)
$5.43 \times 10^{-4}$ (supercooled $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$, Hinckley et al. 1990)
$0.00107,3.23 \times 10^{-4}\left(\mathrm{P}_{\mathrm{GC}}\right.$ by GC-RT correlation with different reference standards, Hinckley et al. 1990)
$\log \mathrm{P}_{\mathrm{L}} / \mathrm{Pa}=12.63-4742 /(\mathrm{T} / \mathrm{K})(\mathrm{GC}-\mathrm{RT}$ correlation, Hinckley et al. 1990)
$2.51 \times 10^{-4}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$(4.11-281) \times 10^{-7} ; 2.76 \times 10^{-5}\left(\mathrm{P}_{\mathrm{S}}\right.$, quoted exptl., effusion; gas saturation, Delle Site 1997)
$3.39 \times 10^{-5} ; 5.29 \times 10^{-5}, 1.48 \times 10^{-5}, 2.57 \times 10^{-5}\left(\mathrm{P}_{\mathrm{S}}\right.$, quoted lit., calculated; GC-RT correlation, Delle Site 1997)
$5.47 \times 10^{-4} ; 3.59 \times 10^{-5}$ (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with
fugacity ratio $F$, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=11.91-4858 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.34-3760 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\log (\mathrm{P} / \mathrm{Pa})=9.683-4246.51 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. from literature data, Shiu \& Ma 2000)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
0.813 (gas stripping-GC, Southworth 1979)
0.102 (headspace solid-phase microextraction (SPME)-GC, Zhang \& Pawliszyn 1993)
1.22* (gas stripping-GC; measured range $4.1-31^{\circ} \mathrm{C}$, Bamford et al. 1999)
$\ln \mathrm{K}_{\mathrm{AW}}=-7986.53 /(\mathrm{T} / \mathrm{K})+19.124, \Delta \mathrm{H}=66.4 \mathrm{~kJ} \mathrm{~mol}^{-1}$, measured range $4.1-31^{\circ} \mathrm{C}$ (gas stripping-GC, Bamford et al. 1999)
$\log \left(\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right)=9.67-2641 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations:
5.61 (Radding et al. 1976)
5.66 (Leo 1986; quoted, Schüürmann \& Klein 1988)
5.79 (HPLC-RT correlation, Wang et al. 1986)
5.91 (recommended, Sangster 1989, 1993)
5.84 (TLC retention time correlation, De Voogt et al. 1990)
5.79 (recommended, Hansch et al. 1995))
$5.54 \pm 0.19,5.50 \pm 0.64$ (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
5.91 (range 5.74-6.04) (shake flask/slow stirring-HPLC/fluorescence, De Maagd et al. 1998)
5.75 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)
5.33; 4.98 (calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2000)
$\log \mathrm{K}_{\mathrm{OW}}=1.238+1216.89 /(\mathrm{T} / \mathrm{K})$; temp range $5-55^{\circ} \mathrm{C}$ (temperature dependence HPLC- $\mathrm{k}^{\prime}$ correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
$9.50 \quad$ (calculated- $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, Wania \& Mackay 1996)
9.54 (calculated, Finizio et al. 1997)

Bioconcentration Factor, $\log$ BCF:
4.56 (Smith et al. 1978; Steen \& Karickhoff 1981)
4.0 (Daphnia pulex, Southworth et al. 1978)
4.0 (fathead minnow, Veith et al. 1979)
4.56, 5.0 (bacteria, Baughman \& Paris 1981)
4.39 (activated sludge, Freitag et al. 1984)
4.0 (Daphnia pulex, correlated as per Mackay \& Hughes 1984, Howell \& Connell 1986)
4.39, 3.50, 2.54 (activated sludge, algae, fish, Freitag et al. 1985)
4.01 (Daphnia magna, Newsted \& Giesy 1987)
4.303, 4266 (calculated-molecular connectivity indices, calculated- $\mathrm{K}_{\mathrm{ow}}$, Lu et al. 1999)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
$4.52 \quad\left(22^{\circ} \mathrm{C}\right.$, suspended particulates, Herbes et al. 1980)
6.30 (sediments average, Kayal \& Connell 1990)
7.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
5.62 (humic acid, HPLC-k' correlation; Nielsen et al. 1997)
5.77 (5.73-5.80), 5.47 (5.44-5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flaskHPLC/UV, de Maagd et al. 1998)
5.20 (soil, calculated-universal solvation model; Winget et al. 2000)
5.63-7.53; 4.50-6.70 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$5.11 ; 6.33,5.84,6.18\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1 / 2}$ :
Volatilization: aquatic fate rate $\mathrm{k}=8 \times 10^{3} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2} \sim 90 \mathrm{~h}$ (Callahan et al. 1979);
half-lives predicted by one compartment model: $\mathrm{t}_{1 / 2}>1000 \mathrm{~h}$ in stream, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
calculated $t_{1 / 2}=500 \mathrm{~h}$ for a river of $1-\mathrm{m}$ deep with water velocity of $0.5 \mathrm{~m} / \mathrm{s}$ and wind velocity of $1 \mathrm{~m} / \mathrm{s}$ (Southworth 1979; quoted, Herbes et al. 1980; Hallett \& Brecher 1984).
Photolysis: aquatic fate rate $\mathrm{k} \sim 6 \times 10^{-5} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=10-50 \mathrm{~h}$ (Callahan et al. 1979)
$t_{1 / 2}=20 \mathrm{~h}$ in stream, $t_{1 / 2}=50 \mathrm{~h}$ in eutrophic pond or lake and $t_{1 / 2}=10 \mathrm{~h}$ in oligotrophic lake, predicated by one compartment model (Smith et al. 1978)
direct photochemical transformation $t_{1 / 2}(c a l c)=0.59 \mathrm{~h}$, computed near-surface water, latitude $40^{\circ} \mathrm{N}$, midday, midsummer and photolysis $\mathrm{t}_{1 / 2}=3.7 \mathrm{~d}$ and 9.2 d in $5-\mathrm{m}$ deep inland water body without and with sedimentwater partitioning, respectively, to top cm of bottom sediment over full summer day, $40^{\circ} \mathrm{N}$ (Zepp \& Schlotzhauer 1979)
$t_{1 / 2}=0.58 \mathrm{~h}$ in aquatics (quoted of EPA Report 600/7-78-074, Haque et al. 1980)
$t_{1 / 2}=0.2 \mathrm{~d}$ for early day in March (Mill et al. 1981);
$\mathrm{k}=1.93 \mathrm{~h}^{-1}$ (Zepp 1980; quoted, Mill \& Mabey 1985)
$\mathrm{k}=13.4 \times 10^{-5} \mathrm{~s}^{-1}$ in early March with $\mathrm{t}_{1 / 2}=5 \mathrm{~h}$ in pure water at 366 nm , in sunlight at $23-28^{\circ} \mathrm{C}$ and $\mathrm{k}=2.28 \times 10^{-5} \mathrm{~s}^{-1}$ at 313 nm with $1 \%$ acetonitrile in filter-sterilized natural water (Mill et al. 1981); $\mathrm{k}=1.39 \mathrm{~h}^{-1}$ for summer midday at $40^{\circ} \mathrm{N}$ latitude (quoted, Mabey et al. 1982)
$t_{1 / 2}=1-3 \mathrm{~h}$, atmospheric and aqueous photolysis half-life, based on measured photolysis rate constant for midday March sunlight on a cloudy day (Smith et al. 1978; quoted, Harris 1982; Howard et al. 1991) and adjusted for approximate summer and winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)
half-lives on different atmospheric particulate substrates (approx. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=4.0 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=2.0 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=38 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985)
first order daytime decay $\mathrm{k}=0.0125 \mathrm{~min}^{-1}$ for soot particles loading of $1000-2000 \mathrm{ng} / \mathrm{mg}$ and $\mathrm{k}=0.0250$ $\mathrm{min}^{-1}$ for soot particles loading of $30-350 \mathrm{ng} / \mathrm{mg}$ (Kamens et al. 1988)
photodegradation $\mathrm{k}=0.0251 \mathrm{~min}^{-1}$ with $\mathrm{t}_{1 / 2}=0.46 \mathrm{~h}$ in ethanol-water $(2: 3, \mathrm{v} / \mathrm{v})$ solution for initial concentration of 12.5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
pseudo-first-order direct photolysis $\mathrm{k}(\operatorname{exptl})=0.0251 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=0.46 \mathrm{~h}$ and the predicted $\mathrm{k}=0.0245 \mathrm{~min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{obs})=0.94 \mathrm{~h}, \mathrm{t}_{1 / 2}($ calc $)=0.89 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)
Photodegradation $\mathrm{k}=5.0 \times 10^{-4} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: half-lives predicted by one compartment model: $t_{1 / 2}=38 \mathrm{~h}$ in stream, eutrophic pond or lake and oligotrophic lake based on peroxy radical concentration of $10^{-9} \mathrm{M}$ (Smith et al. 1978)
aquatic fate rate $\mathrm{k}=5 \times 10^{3} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=38 \mathrm{~h}$ (Callahan et al. 1979);
$t_{1 / 2}=6400 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
$\mathrm{k}=5 \times 10^{8} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $2 \times 10^{4} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}=3.3 \times 10^{-4} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=0.6 \mathrm{~h}$ under natural sunlight conditions; $\mathrm{k}(\mathrm{aq})=.5.0 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=1.6$ d for free-radical oxidation in air-saturated water (NRCC 1983)
photooxidation $\mathrm{t}_{1 / 2}=0.801-8.01 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);
photooxidation $\mathrm{t}_{1 / 2}=77-3850 \mathrm{~h}$ in water, based on measured rate constant for reaction with hydroxyl radical in water (Howard et al. 1991)
Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation: not observed during enrichment procedures (Smith et al. 1978)
no significant degradation in 7 d for an average of three static-flask screening test (Tabak et al. 1981)
$\mathrm{k}=3.3 \times 10^{-3} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=208 \mathrm{~h}$ for mixed bacterial populations in stream sediment (NRCC 1983)
$\mathrm{k}=1.0 \times 10^{-4} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=288 \mathrm{~d} ; \mathrm{k}=4.0 \times 10^{-6} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=20 \mathrm{yr}$ for mixed bacterial populations in oilcontaminated and pristine stream sediments (NRCC 1983)
$\mathrm{k}=0.0026 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=261 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0043 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=162 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
$t_{1 / 2}($ aq.aerobic $)=2448-16320 \mathrm{~h}$, based on aerobic soil dieaway test data at $10-30^{\circ} \mathrm{C}$ (Howard et al. 1991)
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=9792-65280 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation halflife (Howard et al. 1991).
Biotransformation: rate constant estimated to be $1 \times 10^{-10} \mathrm{~mL}^{\mathrm{m}}$ cell ${ }^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
$\mathrm{k}_{1}=669 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.144 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)
$\log \mathrm{k}_{1}=2.83 \mathrm{~h}^{-1}$; $\log \mathrm{k}_{2}=-0.84 \mathrm{~h}^{-1}$ (Daphnia pulex, correlated as per Mackay \& Hughes 1984, Hawker \& Connell 1986)
$\mathrm{k}_{1}=138.6 \mathrm{~mL} \mathrm{~g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0022 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}, P\right.$. hoyi, Landrum 1988)
$\mathrm{k}_{1}=0.72-1.4 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0096 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $t_{1 / 2}=1-3 \mathrm{~h}$, based on estimated photolysis half-life in air (Howard et al. 1991);
$\mathrm{t}_{1 / 2}=4.20 \mathrm{~h}$ under simulated sunlight, $\mathrm{t}_{1 / 2}=1.35 \mathrm{~h}$ in simulated sunlight + ozone $(0.2 \mathrm{ppm}), \mathrm{t}_{1 / 2}=2.88 \mathrm{~h} \mathrm{in}$ dark reaction ozone ( 0.2 ppm ), under simulated atmospheric conditions (Katz et al. 1979)
$\mathrm{t}_{1 / 2}=0.4 \mathrm{~h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant k $=0.0265 \mathrm{~min}^{-1}$ at $1 \mathrm{cal} \mathrm{cm}^{-2} \mathrm{~min}^{-1}, 10 \mathrm{~g} / \mathrm{m}^{3} \mathrm{H}_{2} \mathrm{O}$ and $20^{\circ} \mathrm{C}$ (Kamens et al. 1988).
Surface water: photolysis $\mathrm{t}_{1 / 2}=0.59 \mathrm{~h}$ near surface water, $\mathrm{t}_{1 / 2}=3.7 \mathrm{~d}$ and 9.2 d in $5-\mathrm{m}$ deep water body without and with sediment-water partitioning in full summer day, $40^{\circ} \mathrm{N}$; photosensitized oxygenation $\mathrm{t}_{1 / 2}=2.6 \mathrm{~h}$ at near surface water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
$\mathrm{t}_{1 / 2}=0.20 \mathrm{~d}$ under summer sunlight (Mill \& Mabey 1985);
$\mathrm{t}_{1 / 2}=1-3 \mathrm{~h}$, based on estimated photolysis half-life in water, Howard et al. 1991);
photolysis $\mathrm{t}_{1 / 2}=0.46 \mathrm{~h}$ (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
Groundwater: $t_{1 / 2}=4896-32640 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: The uptake clearance from sediment was $k=(0.005 \pm 0.001) \mathrm{g}$ of dry sediment $\cdot \mathrm{g}^{-1}$ of organism $\cdot \mathrm{h}^{-1}$, and the elimination rate constants $\mathrm{k}=(0.0014 \pm 0006) \mathrm{h}^{-1}$ for amphipod, $P$. hoyi in Lake Michigan sediments at $4^{\circ} \mathrm{C}$ (Landrum 1989);
desorption $t_{1 / 2}=11.1 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $t_{1 / 2}=4-6250$ d (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$\mathrm{t}_{1 / 2}=240 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and 130 d for $50 \mathrm{mg} / \mathrm{kg}$ treatment (Bulman et al. 1987);
biodegradation $\mathrm{k}=0.0026 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=261 \mathrm{~d}$ for Kidman sandy loam soil, and $\mathrm{k}=0.0043 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=162$
d for McLaurin sandy loam soil (Park et al. 1990);
$\mathrm{t}_{1 / 2} \sim 2448-16320 \mathrm{~h}$, based on aerobic die-away test data at $10-30^{\circ} \mathrm{C}$ (Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988).
Biota: depuration $\mathrm{t}_{1 / 2}=9 \mathrm{~d}$ by oysters (Lee et al. 1978);
elimination $\mathrm{t}_{1 / 2}=4.3-17.8 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=7-15.4 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$ from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.39.1
Reported aqueous solubilities of benz[a]anthracene at various temperatures and reported temperature dependence equation

| May 1980 | May et al. 1978b | May et al. 1983 |  | Velapoldi et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| generator column-HPLC | generator column-HPLC | generator column-HPLC |  | generator column-fluo. |  |
| $\mathbf{t / ~}{ }^{\circ} \mathrm{C} \quad \mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{S} / \mathrm{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ |
| 6.90 .00299 | 250.0094 | 6.9 | 0.00299 | 10 | 0.00342 |
| 10.7 0.00378 | 29 0.0.0122 | 10.7 | 0.00378 | 15 | 0.00475 |
| 14.3 0.00479 |  | 11.0 | 0.00361 | 20 | 0.00669 |
| 19.3 0.00633 |  | 14.7 | 0.00558 | 25 | 0.00935 |
| 23.1 0.00837 | temp dependence eq. 1 | 18.1 | 0.00634 | 30 | 0.01297 |
| 29.7 0.0127 | S $\quad \mu \mathrm{g} / \mathrm{kg}$ | 19.3 | 0.00801 |  |  |
|  | a 0.0003 | 23.6 | 0.00838 |  |  |
| temp dependence eq. 1 | b $\quad-0.0031$ | 25.0 | 0.00862 | eq. 2 | mole fraction |
| $\mathrm{S} \quad \mu \mathrm{g} / \mathrm{kg}$ | c 0.1897 | 29.5 | 0.0124 | A | -83.75982 |
| a 0.0003 | d 1.74 | 29.7 | 0.0127 | B | 41884.5 |
| b $\quad-0.0031$ |  |  |  | C | 161.175 |
| c 0.1897 | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=44.81$ |  |  |  |  |
| d | measured between $5-30^{\circ} \mathrm{C}$ |  |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=49.0$ |  |
|  |  |  |  |  | at $25^{\circ} \mathrm{C}$ |
| $\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=44.81$ <br> measured between $5-30^{\circ} \mathrm{C}$ |  |  |  |  |  |

$\mathrm{S} /(\mu \mathrm{g} / \mathrm{kg})=\mathrm{a} \cdot \mathrm{t}^{3}+\mathrm{b} \cdot \mathrm{t}^{2}+\mathrm{c} \cdot \mathrm{t}+\mathrm{d}$
$\ln x=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot \ln (\mathrm{T} / \mathrm{K})$
$\Delta \mathrm{H}_{\mathrm{sol}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=44.81$
measured between $5-30^{\circ} \mathrm{C}$


FIGURE 4.1.1.39.1 Logarithm of mole fraction solubility ( $\ln x$ ) versus reciprocal temperature for benz[a]anthracene.

TABLE 4.1.1.39.2
Reported vapor pressures of benz[a]anthracene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |  |
| :--- | ---: | :--- | ---: |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |

$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| Kelley \& Rice 1964 | Murray et al. 1972 | de Kruif 1980 | Sonnefeld et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: |
| effusion-electrobalance | Knudsen effusion | torsion-, effusion method | generator column-HPLC |  |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathbf{C} \quad \mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{P} / \mathrm{Pa}$ |
| data represented by | data presented by graph and | 98.07 0.1 | 13.81 | $8.05 \times 10^{-5}$ |
|  | eq. $2 \quad \mathrm{P} / \mathrm{atm}$ | 105.21 0.2 | 13.81 | $6.06 \times 10^{-5}$ |
| eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | A 10.045 | 109.51 | 13.81 | $1.13 \times 10^{-5}$ |
| A 11.528 | B 5925 | 112.62 0.4 | 25.1 | $2.66 \times 10^{-5}$ |
| B 5461 | temp range 330-390 K | 115.06 0.5 | 25.1 | $2.56 \times 10^{-5}$ |
| measured range $104-127^{\circ} \mathrm{C}$ |  | 117.09 0.6 | 25.1 | $2.81 \times 10^{-5}$ |
| $\Delta \mathrm{H}_{\text {subl }}\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=104.56$ |  | 118.82 0.7 | 40.12 | $1.39 \times 10^{-4}$ |
|  | $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=113.5$ | 120.32 0.8 | 40.12 | $1.41 \times 10^{-4}$ |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C} \quad 160-161.5$ |  | 121.66 0.9 | 40.12 | $1.36 \times 10^{-4}$ |
|  |  | $122.87 \quad 1.0$ | $40.75$ | $1.31 \times 10^{-4}$ |
|  |  | $25.0 \quad 7.3 \times 10^{-6}$ | 40.85 | $1.17 \times 10^{-4}$ |
|  |  | extrapolated | 40.85 | $1.27 \times 10^{-4}$ |
|  |  |  | 40.85 | $1.21 \times 10^{-4}$ |
| Hoyer \& Peperle 1958 |  | $\Delta \mathrm{H}_{\text {sub }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=113$ | 49.56 | $3.87 \times 10^{-4}$ |
| effusion method |  |  | 49.56 | $3.85 \times 10^{-4}$ |
| $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ |  |  | 49.56 | $3.88 \times 10^{-4}$ |
|  |  |  | 34.93 | $2.69 \times 10^{-4}$ |
| data presented by equation. |  |  | 25.0 | $2.80 \times 10^{-5}$ |

TABLE 4.1.1.39.2 (Continued)

| Kelley \& Rice 1964 |  | Murray et al. 1972 |  | de Kruif 1980 |  | Sonnefeld et al. 1983 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| effusion-electrobalance |  | Knudsen effusion |  | torsion-, effusion method |  | generator column-HPLC |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| eq. 1 | $\mathrm{P} / \mathrm{mmHg}$ |  |  |  |  | eq. 1 | P/Pa |
| A | 13.68 |  |  |  |  | A | 9.684 |
| B | 6250 |  |  |  |  | B | 4246.51 |
| for temp range $60-120^{\circ} \mathrm{C}$ |  |  |  |  |  | $\Delta \mathrm{H}_{\text {subl }}$ <br> for tem | $\begin{aligned} & \left.{ }^{1}\right)=51.83 \\ & 10-50^{\circ} \mathrm{C} \end{aligned}$ |



FIGURE 4.1.1.39.2 Logarithm of vapor pressure versus reciprocal temperature for benz[a]anthracene.

## TABLE 4.1.1.39.3

Reported Henry's law constants of benz[a]anthracene at various temperatures and temperature dependence equations
$\ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1) $\quad \log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(2) $\quad \log \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(4) $\quad \ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{T} / \mathrm{K})^{2}$

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| gas stripping-GC/MS |  |  |
| :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathbf{m o l}\right)$ |
|  |  |  |
| 4.1 | $0.10,0.22$ | average |
| 11.0 | $0.24,0.41$ | 0.15 |
| 18.0 | $0.50,0.79$ | 0.31 |
| 25.0 | $0.91,1.64$ | 0.63 |
| 31.0 | $1.43,3.13$ | 1.22 |
| $\ln \mathrm{~K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | 2.11 |  |

TABLE 4.1.1.39.3 (Continued)
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| gas stripping-GC/MS |  |  |
| :--- | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathrm{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathrm{mol}\right)$ | $\mathbf{H} /\left(\mathbf{P a ~ m}^{3} / \mathrm{mol}\right)$ |
| A | 19.124 |  |
| B | 7986.5 |  |
| enthalpy, entropy change: |  |  |
| $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=66.4 \pm 6.9$ <br> $\Delta \mathrm{~S} /\left(\mathrm{J} \cdot \mathrm{K}^{-1} \mathrm{~mol}^{-1}\right)=159$ <br>  |  |  |



FIGURE 4.1.1.39.3 Logarithm of Henry's law constant versus reciprocal temperature for benz[a]anthracene.

### 4.1.1.40 Benzo[b]fluoranthene



Common Name: Benzo[b]fluoranthene
Synonym: 2,3-benzofluoranthene, 3,4-benzofluoranthene, benz[e]acephenanthrylene, B $[b] F$
Chemical Name: 2,3-benzofluoranthene
CAS Registry No: 205-99-2
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{12}$
Molecular Weight: 252.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
168 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
481 (Bjørseth 1983)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
222.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999) 268.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 56.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0395 ( mp at $168^{\circ} \mathrm{C}$ )
Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
0.0015 (generator column-HPLC/fluorescence, Wise et al. 1981)
0.0015 (average lit. value, Pearlman et al. 1984)
0.00109 (generator column-HPLC/fluo., De Maagd et al. 1998) $\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-0.351-1303 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$6.67 \times 10^{-5}\left(20^{\circ} \mathrm{C}\right.$, estimated, Callahan et al. 1979)
$2.12 \times 10^{-5}$ (Yamasaki et al. 1984)
$5.0 \times 10^{-8} ; 1.30 \times 10^{-6}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992 ; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.43-5880 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.48-4578 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
$7.55 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4682 /(\mathrm{T} / \mathrm{K})+10.58, \Delta \mathrm{H}_{\text {vap. }}=-89.7 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations.):
$0.051 \quad\left(20^{\circ} \mathrm{C}\right.$, gas stripping-HPLC/fluorescence, measured range $10-55^{\circ} \mathrm{C}$, ten Hulscher et al. 1992) $\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=9.83-3274 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
$0.0485 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=2.955-2245 /(\mathrm{T} / \mathrm{K})$, (van’t Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
5.78 (HPLC-RT correlation, Wang et al. 1986)
5.78 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ :
5.15 (microorganisms-water, Mabey et al. 1982)
$4.00 \quad$ (Daphnia magna, Newsted \& Giesy 1987)
0.959, 0.230 (Polychaete sp, Capitella capitata, Bayona et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
6.182; 6.00, 6.18 (sediment: conen ratio $\mathrm{C}_{\text {sed }} / \mathrm{C}_{\mathrm{W}}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter \& Alden 1994)
$5.45 \quad\left(\log \mathrm{~K}_{\mathrm{DOC}}-\right.$ Aldrich humic acid, RP-HPLC, Ozretich et al. 1995)
$6.57 \quad\left(10^{\circ} \mathrm{C}\right), 6.55,6.61\left(20^{\circ} \mathrm{C}\right), 6.26\left(35^{\circ} \mathrm{C}\right), 6.44,6.45\left(45^{\circ} \mathrm{C}\right)\left(\log \mathrm{K}_{\mathrm{DOC}}\right.$, dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers \& ten Hulscher 1996)
$6.20 \quad\left(20^{\circ} \mathrm{C}, \log \mathrm{K}_{\mathrm{DOC}}\right.$, particulate organic material from lake, Lüers \& ten Hulscher 1996)
6.15-8.02; 5.70-7.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001, for benzo $[b+j+k]$ fluoranthenes)
$5.91 ; 6.50,6.26,6.68\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001, for benzo $[b+j+k]$ fluoranthenes)

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1 / 2}$ :
Volatilization:
Photolysis: atmospheric and aqueous $\mathrm{t}_{1 / 2}=8.7-720 \mathrm{~h}$, based on measured rate of photolysis in heptane irradiated with light $>290 \mathrm{~nm}$ (Howard et al. 1991);
first order daytime decay rate constants: $\mathrm{k}=0.0065 \mathrm{~min}^{-1}$ for $1000-2000 \mathrm{ng} / \mathrm{mg}$ soot particles loading and $\mathrm{k}=0.0090 \mathrm{~min}^{-1}$ with $30-350 \mathrm{ng} / \mathrm{mg}$ loading (Kamens et al. 1988);
$\mathrm{t}_{1 / 2}(\mathrm{obs})=.4.31 \mathrm{~h}, \mathrm{t}_{1 / 2}(\mathrm{calc})=1.49 \mathrm{~h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
Photodegradation $\mathrm{k}=3 \times 10^{-5} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002).
Oxidation: rate constant $k=4 \times 10^{7} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=5 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982);
photooxidation $\mathrm{t}_{1 / 2}=1.43-14.3 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).
Hydrolysis: not hydrolyzable (Mabey et al. 1982; no hydrolyzable groups (Howard et al. 1991).
Biodegradation:
aerobic $t_{1 / 2}=8640-14640 \mathrm{~h}$, based on aerobic soil die-away test data (Coover \& Sims 1987; quoted, Howard et al. 1991);
$\mathrm{k}=0.0024 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=294 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0033 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=211 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990);
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=34560-58560 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991).
Biotransformation: estimated to be $3 \times 10^{-12} \mathrm{~mL}$ cell ${ }^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=0.11-0.38 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0029 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Sorption-Desorption Rate constants: desorption rate constant $\mathrm{k}=0.016 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=42.4 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=1.43-14.3 \mathrm{~h}$, based on estimated photooxidation half-life in air (Howard et al. 1991)
half-lives under simulated atmospheric conditions: simulated sunlight $-t_{1 / 2}=8.70 \mathrm{~h}$, simulated sunlight + ozone $(0.2 \mathrm{ppm}) \mathrm{t}_{1 / 2}=4.20 \mathrm{~h}$, dark reaction ozone $(0.2 \mathrm{ppm}) \mathrm{t}_{1 / 2}=52.70 \mathrm{~h}$ (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983);
$\mathrm{t}_{1 / 2}=1.3 \mathrm{~h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant k $=0.0091 \mathrm{~min}^{-1}$ at $1 \mathrm{cal} \mathrm{cm}^{-2} \mathrm{~min}^{-1}, 10 \mathrm{~g} / \mathrm{m}^{3} \mathrm{H}_{2} \mathrm{O}$ and $20^{\circ} \mathrm{C}$ (Kamens et al. 1988).
Surface water: $\mathrm{t}_{1 / 2}=8.7-720 \mathrm{~h}$, based on estimated aqueous photolysis half-life (Lane \& Katz 1977; Muel \& Saguem 1985; quoted, Howard et al. 1991).

Groundwater: $\mathrm{t}_{1 / 2}=17280-29280 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: desorption $\mathrm{t}_{1 / 2}=42.4 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: biodegradation rate constant $\mathrm{k}=0.0024 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=294 \mathrm{~d}$ for Kidman sandy loam soil, and $\mathrm{k}=0.0033$ $\mathrm{d}^{-1}$ with $\mathrm{t}_{1 / 2}=211 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$\mathrm{t}_{1 / 2}=8640-14640 \mathrm{~h}$, based on aerobic die-away test data (Coover \& Sims 1987; quoted, Howard et al. 1991); $\mathrm{t}_{1 / 2}=42 \mathrm{wk}, 9.0 \mathrm{yr}$ (quoted, Luddington soil, Wild et al. 1991).
Biota: elimination $\mathrm{t}_{1 / 2}=5.7-16.9 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=7.7 \mathrm{~d}$ from Oyster (isomer unspecified), $\mathrm{t}_{1 / 2}=3.9 \mathrm{~d}$ from clam Mercenario mercenaria (isomer unspecified) (quoted, Meador et al. 1995).

### 4.1.1.41 Benzo[j]fluoranthene



Common Name: Benzo[j]fluoranthene
Synonym: 7,8-benzofluoranthene, 10,11-fluoranthene
Chemical Name: benzo[j]fluoranthene
CAS Registry No: 205-82-3
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{12}$
Molecular Weight: 252.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
166 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
480 (Bjørseth 1983)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
222.8 (Ruelle \& Kesselring 1997)
268.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0414 (mp at $166^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0025 (generator column-HPLC/fluorescence, Wise et al. 1981)
0.0025 (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
6.44 (calculated-MCI $\chi$ as per Rekker \& De Kort 1979, Ruepert et al. 1985)
6.40 (Bayona et al. 1991)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
0.914; -0.222 (Polychaete sp, Capitella capitata, Bayona et al. 1991)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
6.15-8.02; 5.70-7.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001, for benzo $[b+j+k]$ fluoranthenes)
5.91; $6.50,6.26,6.68\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001, for benzo $[b+j+k] f l u o r a n t h e n e s)$

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Biota: elimination $\mathrm{t}_{1 / 2}=7.7 \mathrm{~d}$ from Oyster (isomer unspecified), $\mathrm{t}_{1 / 2}=3.9 \mathrm{~d}$ from clam Mercenario mercenaria (isomer unspecified) (quoted, Meador et al. 1995).

### 4.1.1.42 Benzo[k]fluoranthene



Common Name: Benzo[k]fluoranthene
Synonym: 8,9-benzofluoranthene, 11,12-benzofluoranthene, B[k]F
Chemical Name: 8,9-benzofluoranthene
CAS Registry No: 207-08-9
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{12}$
Molecular Weight: 252.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
217 (Weast 1977; Bjørseth 1983; Stephenson \& Malanowski 1987; Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
480 (Stephenson \& Malanowski 1987; Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
222.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999)
268.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
56.6 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right)$, $\mathrm{F}: 0.0131\left(\mathrm{mp}\right.$ at $\left.217^{\circ} \mathrm{C}\right)$ 0.0126 (calculated, Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
0.0008 (generator column-HPLC/UV, Wise et al. 1981)
0.00081 (average lit. value, Pearlman et al. 1984)
0.00109 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-0.351-1448 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$1.28 \times 10^{-8}\left(20^{\circ} \mathrm{C}\right.$, Radding et al. 1976)
$6.70 \times 10^{-5}\left(20^{\circ} \mathrm{C}\right.$, Mabey et al. 1982)
$2.07 \times 10^{-5}($ Yamasaki et al. 1984)
$5.20 \times 10^{-8}, 4.93 \times 10^{-6}\left(20^{\circ} \mathrm{C}\right.$, lit. mean solid $\mathrm{P}_{\mathrm{S}}$, supercooled liquid value $\mathrm{P}_{\mathrm{L}}$, Bidleman \& Foreman 1987)
$1.29 \times 10^{-7}$ (extrapolated, Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.8907-6792 /(\mathrm{T} / \mathrm{K})$; temp range 363-430 K (Antoine eq., Stephenson \& Malanowski 1987)
$2.09 \times 10^{-5}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$5.20 \times 10^{-8} ; 4.14 \times 10^{-6}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with
fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.43-5874 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.48-4427 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$8.96 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4623 /(\mathrm{T} / \mathrm{K})+10.46 ; \Delta \mathrm{H}_{\text {vap }}=-88.5 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant $\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right.$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$0.111 \quad\left(15^{\circ} \mathrm{C}\right.$, calculated, Baker \& Eisenreich 1990)
$0.043^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, gas stripping-HPLC/fluorescence, measured range $10-55^{\circ} \mathrm{C}$, ten Hulscher et al. 1992)
$\log (\mathrm{H} /(\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}))=9.83-2979 /(\mathrm{T} / \mathrm{K})$ (Passivirta et al. 1999)
$0.0422 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured values, Staudinger \& Roberts 1996 , 2001)
$\log \mathrm{K}_{\mathrm{AW}}=3.498-2421 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
6.84 (calculated-fragment const., Callahan et al. 1979)
6.06 (calculated-f const., Mabey et al. 1982)
$6.44 \quad$ (calculated-MCI $\chi$ as per Rekker \& De Kort 1979)
$6.40 \quad$ (Bayona et al. 1991)
6.50 (calculated-S and mp, Capel et al. 1991)
7.20 (calculated- $\mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)
6.00 (selected, Mackay et al. 1992; quoted, Finizio et al. 1997)
6.30 (computed-expert system SPARC, Kollig 1995)
6.50-6.85; 6.73
(quoted lit. range; lit. mean, Meador et al. 1995)
6.11
(range 5.86-6.28) (shake flask/slow stirring-HPLC/fluo., De Maagd et al. 1998)
5.94; 6.16
(quoted lit.; calculated, Passivirta et al. 1999)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
11.19 (calculated, Finizio et al. 1997)

Bioconcentration Factor, $\log$ BCF:
5.15 (microorganisms-water, calculated from $\mathrm{K}_{\mathrm{OW}}$, Mabey et al. 1982)
4.12 (Daphnia magna, Newsted \& Giesy 1987)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
5.99 (sediments average, Kayal \& Connell 1990)
7.00 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
$6.80\left(10^{\circ} \mathrm{C}\right), 6.74,6.89\left(20^{\circ} \mathrm{C}\right), 6.46\left(35^{\circ} \mathrm{C}\right), 6.44,6.45\left(45^{\circ} \mathrm{C}\right)\left(\log \mathrm{K}_{\mathrm{DOC}}\right.$ - dissolved organic material from lake, gas-purge technique- HPLC/fluorescence, Lüers \& ten Hulscher 1996)
$6.30 \quad\left(20^{\circ} \mathrm{C}, \log \mathrm{K}_{\mathrm{POC}}-\right.$ particulate organic material from lake, Lüers \& ten Hulscher 1996)
6.04 (5.93-6.12), 5.47 (5.39-5.54) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flaskHPLC/UV, de Maagd et al. 1998)
6.15-8.02; 5.70-7.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001, for benzo $[b+j+k]$ fluoranthenes)
$5.91 ; 6.50,6.26,6.68\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2 , 3 -solvophobic approach, Krauss \& Wilcke 2001, for benzo $[b+j+k]$ fluoranthenes)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: atmospheric and aqueous photolysis $t_{1 / 2}=3.8-499 \mathrm{~h}$, based on measured rate of photolysis in heptane under November sunlight and adjusted by ratio of sunlight photolysis half-lives in water versus heptane (Howard et al. 1991);
first-order daytime decay constants: $\mathrm{k}=0.0047 \mathrm{~min}^{-1}$ for soot particles loading of $1000-2000 \mathrm{ng} / \mathrm{mg}$ and $\mathrm{k}=0.0013 \mathrm{~min}^{-1}$ with $30-350 \mathrm{ng} / \mathrm{mg}$ loading (Kamens et al. 1988);
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{obs})=0.88 \mathrm{~h}, \mathrm{t}_{1 / 2}(\mathrm{calc})=0.80 \mathrm{~h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Photodegradation $\mathrm{k}=3 \times 10^{-5} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant $\mathrm{k}=4 \times 10^{7} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=5 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982);
photooxidation $t_{1 / 2}=1.1-11 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).
Hydrolysis: not hydrolyzable (Mabey et al. 1982);
no hydrolyzable groups (Howard et al. 1991).
Biodegradation:
aerobic $\mathrm{t}_{1 / 2}=21840-51360 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991);
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) $=87360-205440 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation halflife (Howard et al. 1991).

Biotransformation: estimated to be $3 \times 10^{-12} \mathrm{~mL} \mathrm{cell}^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=1.1-11 \mathrm{~h}$, based on estimated photooxidation half-life in air (Howard et al. 1991);
$\mathrm{t}_{1 / 2}=14.10 \mathrm{~h}$ in simulated sunlight: $\mathrm{t}_{1 / 2}=3.90 \mathrm{~h}$ in simulated sunlight + ozone $(0.2 \mathrm{ppm}), \mathrm{t}_{1 / 2}=34.90 \mathrm{~h}$ in dark reaction ozone ( 0.2 ppm ) u) under simulated atmospheric conditions (Katz et al. 1979);
$t_{1 / 2}=0.8 \mathrm{~h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $\mathrm{k}=0.0138 \mathrm{~min}^{-1}$ at $1 \mathrm{cal} \mathrm{cm}^{-2} \mathrm{~min}^{-1}$ and $10 \mathrm{~g} / \mathrm{m}^{3} \mathrm{H}_{2} \mathrm{O}$ at $20^{\circ} \mathrm{C}$ (Kamens et al. 1988).
Surface water: $\mathrm{t}_{1 / 2}=3.8-499 \mathrm{~h}$, based on photolysis half-life in water (Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=42680-102720 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: desorption $t_{1 / 2}=23.2 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $t_{1 / 2}=21840-51360 \mathrm{~h}$, based on aerobic soil die-away test data Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
mean $\mathrm{t}_{1 / 2}=8.7 \mathrm{yr}$ for Luddington soil (Wild et al. 1991).
Biota: elimination $\mathrm{t}_{1 / 2}=11.9 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=7.7 \mathrm{~d}$ from Oyster (isomer unspecified), $\mathrm{t}_{1 / 2}=3.9 \mathrm{~d}$ from clam Mercenario mercenaria (isomer unspecified) (quoted, Meador et al. 1995).

TABLE 4.1.1.42.1
Reported Henry's law constants of benzo[k]fluoranthene at various temperatures and temperature dependence equations

$$
\begin{aligned}
& \ln \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \ln \left(1 / \mathrm{K}_{\mathrm{AW}}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \ln \left(\mathrm{k}_{\mathrm{H}} / \mathrm{atm}\right)=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \ln \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{~m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \\
& \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} \cdot(\mathrm{~T} / \mathrm{K})+\mathrm{C} \cdot(\mathrm{~T} / \mathrm{K})^{2}
\end{aligned}
$$

$$
\begin{equation*}
\log \mathrm{K}_{\mathrm{AW}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K}) \tag{1}
\end{equation*}
$$

$\log \left(1 / K_{\text {AW }}\right)=A-B /(T / K)$
$\ln \left[\mathrm{H} /\left(\mathrm{atm} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\right]=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
ten Hulscher et al. 1992

| gas stripping-HPLC/fluorescence |  |
| :---: | :---: |
| t/ ${ }^{\circ} \mathrm{C}$ | H/( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ) |
| 10.0 | 0.022 |
| 20.0 | 0.043 |
| 35.0 | 0.107 |
| 40.1 | 0.138 |
| 45.0 | 0.198 |
| 55.0 | 0.403 |
| $\ln \mathrm{K}_{\mathrm{AW}}=-\Delta \mathrm{H}_{\mathrm{vol}} / \mathrm{RT}+\Delta \mathrm{S}_{\mathrm{vol}} / \mathrm{R}$$\mathrm{R}=8.314 \mathrm{~Pa} \mathrm{~m}^{3} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}$ |  |
|  |  |
| $\Delta \mathrm{S}_{\text {vol }}$ | 16.41 |
| $\Delta \mathrm{H}_{\text {vol }} \quad 5893.7$ |  |
|  |  |
| $\Delta \mathrm{H}_{\text {vol }} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=49 \pm 1.9$entropy of volatilization, $\Delta \mathrm{S}$ |  |
| $\mathrm{T} \Delta \mathrm{S}_{\mathrm{vol}} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=40 \pm 4$ |  |

at $20^{\circ} \mathrm{C}$


FIGURE 4.1.1.42.1 Logarithm of Henry's law constant versus reciprocal temperature for benzo[k]fluoranthrene.

### 4.1.1.43 Benzo[a]pyrene



Common Name: Benzo[a]pyrene
Synonym: BaP, B (a)P, 3,4-benzopyrene
Chemical Name: benzo $[a$ ]pyrene
CAS Registry No: 50-32-8
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{12}$
Molecular Weight: 252.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
181.1 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
495 (Stephenson \& Malanowski 1987; Dean 1992)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
222.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999)
262.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
17.324 (Ruelle \& Kesselring 1997)
8.49, 17.32; 25.61 ( $117.05,181.05^{\circ} \mathrm{C}$; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
38.5 (differential scanning calorimetry, Hinckley et al. 1990)
21.77, 38.13 (117.05, $181.05^{\circ} \mathrm{C}$, Chickos et al. 1999)
42.35, 43.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
38.2 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.0294 ( mp at $181.1^{\circ} \mathrm{C}$ )
0.0903 (calculated, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$0.004 \quad\left(27^{\circ} \mathrm{C}\right.$, nephelometry, Davis et al. 1942)
0.0043 (shake flask-UV/fluorescence, Barone et al. 1967)
0.0061 (average, Barone et al. 1967)
$0.0005 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
$0.000038,0.0000606,0.000038,0.0000505$ (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)
0.00121 (Haque \& Schmedding 1975)
0.0038 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.0002 (Rossi 1977; Neff 1979)
0.0012 (generator column-HPLC, Wise et al. 1981)
$0.00162^{*}$ (generator column-HPLC, measured range $10-30^{\circ} \mathrm{C}$, May et al. 1983)
0.00158* (generator column-spectrofluorimetry, measured range $10-30^{\circ} \mathrm{C}$, Velapoldi et al. 1983)
0.0038 (selected value, Pearlman et al. 1984)
0.00154* (generator column-HPLC/UV, measured $8.0-25.0^{\circ} \mathrm{C}$, Whitehouse 1984)
0.0016 (generator column-HPLC/UV, Billington et al. 1988)
0.000504 (shake flask-LSC, Eadie et al. 1990)
0.00472 (shake flask-fluorescence, Haines \& Sandler 1995)
0.00182 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
$0.00622 \pm 0.00023 ; 0.0038,0.0018 \pm 0.0003$ (shake flask-SPME (solid-phase micro-extraction)-GC; quoted lit. values; Paschke et al. 1999)
$\log \mathrm{S}_{\mathrm{L}}(\mathrm{mol} / \mathrm{L})=-1.310-906.6 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=-2.59638-6046.87 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$7.32 \times 10^{-7}$ (effusion method, extrapolated, Murray et al. 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=9.601-6181 /(\mathrm{T} / \mathrm{K})$; temp range $358-431 \mathrm{~K}$ (Knudsen effusion method, Murray et al. 1974)
$1.12 \times 10^{-4}, 1.50 \times 10^{-5}\left(\mathrm{P}_{\mathrm{GC}}\right.$, GC-RT correlation with different GC columns, Bidleman 1984)
$2.35 \times 10^{-5}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with $\Delta \mathrm{S}_{\text {fus }}$ Bidleman 1984)
$1.22 \times 10^{-5}$ (Yamasaki et al. 1984)
$3.2 \times 10^{-7}, 1.23 \times 10^{-5}$ (lit. mean, supercooled liq. value, Bidleman \& Foreman 1987)
$7.51 \times 10^{-7}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.6067-6181 /(\mathrm{T} / \mathrm{K})$; temp range $358-431 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$1.12 \times 10^{-4}, 7.24 \times 10^{-5}\left(\mathrm{P}_{\mathrm{GC}}\right.$, GC-RT correlation with different reference standards, Hinckley et al. 1990)
$2.35 \times 10^{-5}, 7.28 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with different $\Delta \mathrm{S}_{\text {fus }}$ Hinckley et al. 1990)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=11.59-4989 /(\mathrm{T} / \mathrm{K})$ (liquid phase, GC-RT correlation, Clausius-Clapeyron eq., Hinckley et al. 1990) $1.17 \times 10^{-5}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calculated from Yamasaki et al 1984, Finizio et al. 1997)
$7.51 \times 10^{-7}, 7.45 \times 10^{-7}$ (quoted exptl., effusion, Delle Site 1997)
$7.01 \times 10^{-7} ; 3.51 \times 10^{-6}, 4.73 \times 10^{-7}, 2.25 \times 10^{-7}$ (quoted lit., calculated-UNIFAC; GC-RT correlation, Delle Site 1997)
$1.54 \times 10^{-5} ; 1.39 \times 10^{-6}$ (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio $F$, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.17-5371 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=10.71-4465 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
$5.90 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4755 /(\mathrm{T} / \mathrm{K})+10.72 ; \Delta \mathrm{H}_{\text {vap }} .=-91.0 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.009 \quad\left(15^{\circ} \mathrm{C}\right.$, calculated, Baker \& Eisenreich 1990)
$0.0079 \quad\left(10^{\circ} \mathrm{C}\right.$, estimated, McLachlan et al. 1990)
$0.034^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, gas stripping-HPLC/fluorescence, measured range $10-55^{\circ} \mathrm{C}$, ten Hulscher et al. 1992)
0.074 (wetted wall column-GC, Altschuh et al. 1999)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=12.02-3558 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
$0.035 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured values, Staudinger \& Roberts 1996, 2001)
$\log \mathrm{K}_{\mathrm{AW}}=1.732-1927 /(\mathrm{T} / \mathrm{K})($ van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
6.04 (Radding et al. 1976)
6.31 (Smith et al. 1978)
5.99, 5.78 (calculated-fragment const., Hansch \& Leo 1979)
6.34 (Steen \& Karickhoff 1981)
6.50 (RP-TLC-k' correlation, Bruggeman et al. 1982)
6.20 (shake flask-GC, Hanai et al. 1982)
5.85-5.12; 5.88-6.04; 5.99, $6.00 \pm 0.1\left(23^{\circ} \mathrm{C}\right.$, shake flask- concentration ratio/UV spec.; shake flask-HPLC/UV;
exptl. mean value, recommended value; Mallon \& Harris 1984)
6.74, 7.77, 7.99 (HPLC-RT correlation, Sarna et al. 1984)
6.42 (HPLC-RT correlation, Rapaport et al. 1984)
5.97 (Hansch \& Leo 1985)
6.78 (HPLC-RT correlation, Webster et al. 1985)
6.04 (HPLC-RT correlation, Wang et al. 1986)
6.44 (TLC retention time correlation, De Voogt et al. 1990)
6.35 (recommended, Sangster 1993)
5.97 (recommended, Hansch et al. 1995)
$6.02 \pm 0.19,6.14 \pm 0.71$ (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
6.13 (5.91-6.28) (slow stirring-HPLC/fluorescence, De Maagd et al. 1998)
6.27 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
$10.80 \quad$ (calculated- $\mathrm{K}_{\mathrm{OW}} / \mathrm{K}_{\mathrm{AW}}$, Wania \& Mackay 1996)
10.77 (calculated, Finizio et al. 1997)

Bioconcentration Factor, $\log$ BCF:
1.09; 2.22; $3.45 \quad$ (steady-state, bluegills; midge larva; periphyton, Leversee et al. 1981)
$4.74 \quad$ (P. hoyi, Eadie et al. 1982)
3.90 (Daphnia magna, McCarthy 1983)
3.69, 4.45 (Lepomis macrochirus, bluegill sunfish, Spacie et al., 1983)
$4.00 \quad$ (activated sludge, Freitag et al. 1984)
3.42 (bluegills, McCarthy \& Jimenez 1985)
2.35, 2.45 (bluegills-with dissolved humic material, McCarthy \& Jimenez 1985)
2.68, 3.52, $4.0 \quad$ (fish, algae, activated sludge, Freitag et al. 1985)
3.51
(worms, Frank et al. 1986)
6.95, 6.51 ( $P$. hoyi of Lake Michigan interstitial waters, Landrum et al. 1985)
3.34 (P. hoyi of Government Pond of Grand Haven in Michigan, Landrum et al. 1985)
2.69 (Gobas et al. 1987)
$4.11 \quad$ (Daphnia magna, Newsted \& Giesy 1987)
$3.77 \quad\left(10-20^{\circ} \mathrm{C}\right.$, H. limbata, Landrum \& Poore 1988)
4.61, 3.86, $3.87 \quad\left(4^{\circ} \mathrm{C}\right.$, P. hoyi, S. heringianus, Mysis relicta, Landrum \& Poore 1988)
4.69, 3.93 (calculated for amphipods and mysids, Evans \& Landrum 1989)
3.22-3.59; 2.96-3.32 (Daphnia magna in natural waters with humic substances, measured range; predicted range, Kokkonen et al. 1989)
1.140, -0.155 (Polychaete sp, Capitella capitata, Bayona et al. 1991)
6.22, 6.04; 3.68, 5.01, 4.90, 5.15(oligochaetes; chironomid larvae, Bott \& Standley 2000)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
5.95 (Aldrich humic acid, RP-HPLC separation, Landrum et al. 1984)
4.59, 4.72, 4.26 (humic materials in natural water: Huron River $6.1 \%$ OC winter, Grand River 10.7\% DOC spring, Lake Michigan $5.5 \%$ DOC spring, RP-HPLC separation method, Landrum et al. 1984)
6.66 (LSC, Eadie et al. 1990)
6.26 (sediments average, Kayal \& Connell 1990)
8.30 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
7.0 (Rotterdam Harbor sediment $4.6 \%$ OC, batch sorption equilibrium, Hegeman et al. 1995)
6.00, 6.28, 6.17; 5.81 (marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island; quoted lit., McGroddy \& Farrington 1995)
5.93 (Aldrich humic acid, Ozretich et al. 1995)
$6.54\left(10^{\circ} \mathrm{C}\right), 6.46,6.60\left(20^{\circ} \mathrm{C}\right), 6.14\left(35^{\circ} \mathrm{C}\right), 6.07,6.09\left(45^{\circ} \mathrm{C}\right)\left(\log \mathrm{K}_{\mathrm{DOC}}\right.$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers \& ten Hulscher 1996)
$6.30\left(20^{\circ} \mathrm{C}, \log \mathrm{K}_{\mathrm{POC}}-\right.$ particulate organic material from lake, Lüers \& ten Hulscher 1996)
6.27; 6.30 (humic acid, HPLC-k' correlation; quoted lit., Nielsen et al. 1997)
$5.72,5.89,5.51(\mathrm{pH} 5,6.5,8$, humic acid from sediments of River Arno, De Paolis \& Kukkonen 1997)
4.81, 4.87, 4.49 ( $\mathrm{pH} 5,6.5,8$, fulvic acid from sediments of River Arno, De Paolis \& Kukkonen 1997)
$5.54,5.59,5.37(\mathrm{pH} 5,6.5,8, \mathrm{HA}+\mathrm{FA}$ extracted from sediments of River Arno, De Paolis \& Kukkonen 1997)
$5.51,5.74,5.68$ (pH 5, 6.5, 8, HA extracted from sediments of Tyrrenhian Sea, De Paolis \& Kukkonen 1997)
4.93, 4.84, 4.85 (pH 5, 6.5, 8, FA extracted from sediments of Tyrrenhian Sea, De Paolis \& Kukkonen 1997)
$5.66,5.46,5.60(\mathrm{pH} 5,6.5,8, \mathrm{HA}+$ FA from sediments of Tyrrenhian Sea, De Paolis \& Kukkonen 1997)
5.22, 5.46, 5.60 (pH 5, 6.5, 8, HA extracted from water of River Arno, De Paolis \& Kukkonen 1997)
4.67, 4.80, $4.45(\mathrm{pH} 5,6.5,8$, FA extracted from water of River Arno, De Paolis \& Kukkonen 1997)
$5.21,5.29,5.18$ (pH 5, 6.5, 8, HA + FA extracted from water of River Arno, De Paolis \& Kukkonen 1997)
4.62, 4.52, 4.61 ( $\mathrm{pH} 5,6.5,8$, FA extracted from water of Tyrrenhian Sea, De Paolis \& Kukkonen 1997)
5.99 (5.92-6.04), 5.53 (5.43-5.61) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flaskHPLC/UV, de Maagd et al. 1998)
5.25-6.18 (Lake Michigan sediment, Kukkonen \& Landrum 1998)
5.48-5.69, 5.56, 5.55, 5.49, $5.30\left(\log \mathrm{~K}_{\mathrm{Doc}}\right.$ : humic acid from Lake Hohlohsee in Black Forest, soil leachate, fulvic acid from brown coal-derived production effluent, fulvic acid from groundwater, fulvic acid from effluent of a waste water plant near Karlsruhe, Haitzer et al. 1999)
5.53 (Clay Creek sediment with organic matter content $0.45 \%$, Bott \& Standley. 2000)
6.23 (sediment: organic carbon OC $-0.5 \%$, average, Delle Site 2001)
6.39-8.17; 6.30-8.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
3.12; 6.67, $6.58,6.79\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium method, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss \& Wilcke 2001)
6.15; 6.34 (Plym river sediment; plym sea sediment, batch equilibrium-LSC, Turner \& Rawling 2002)
6.49; 6.31 (Carnon river sediment; Carnon sea sediment, batch equilibrium-LSC, Turner \& Rawling 2002)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: aquatic fate rate of $300 \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=22 \mathrm{~h}$ (Callahan et al. 1979); half-lives predicted by one compartment model: $t_{1 / 2}=140 \mathrm{~h}$ in river water, $\mathrm{t}_{1 / 2}=350 \mathrm{~h}$ in eutrophic pond, $\mathrm{t}_{1 / 2}=700 \mathrm{~h}$ in eutrophic lake and oligotrophic lake (Smith et al. 1978);
calculated $\mathrm{t}_{1 / 2}=1500 \mathrm{~h}$ for a river of $1-\mathrm{m}$ deep with water velocity of $0.5 \mathrm{~m} \mathrm{~s}^{-1}$ and wind velocity of $1 \mathrm{~m} / \mathrm{s}$ (Southworth 1979; Herbes et al. 1980);
sublimation rate constant from glass surface of $<1 \times 10^{-5} \mathrm{~s}^{-1}$ was measured at $24^{\circ} \mathrm{C}$ at an airflow rate of 3 L/min (Cope \& Kalkwarf 1987).
Photolysis: photolysis $\mathrm{t}_{1 / 2}=2 \mathrm{~h}$ in methanol solution when irradiated at 254 nm (Lu et al. 1977);
$\mathrm{k}=0.58 \mathrm{~h}^{-1}$ for winter at midday at $40^{\circ} \mathrm{N}$ latitude (Smith et al. 1978);
direct photochemical transformation $\mathrm{t}_{1 / 2}(\mathrm{calc})=0.54 \mathrm{~h}$, computed near-surface water, latitude $40^{\circ} \mathrm{N}$, midday, midsummer and photolysis $\mathrm{t}_{1 / 2}=3.2 \mathrm{~d}$ and 13 d in $5-\mathrm{m}$ deep inland water body without and with sedimentwater partitioning, respectively, to top cm of bottom sediment over full summer day, $40^{\circ} \mathrm{N}$ (Zepp \& Schlotzhauer 1979)
$\mathrm{k}(\mathrm{aq})=.2.8 \times 10^{-4} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1-2 \mathrm{~h}$ (Callahan et al. 1979)
photolytic $\mathrm{t}_{1 / 2}(\mathrm{aq})=0.53 \mathrm{~h}$ (quoted of EPA Report 600/7-78-074, Haque et al. 1980)
$\mathrm{k}=1.30 \mathrm{~h}^{-1}$ (Zepp 1980)
half-lives predicted by one compartment model: $t_{1 / 2}=3.0 \mathrm{~h}$ in river water based on the photolysis rates estimated for summer sunlight, $\mathrm{t}_{1 / 2}=7.5 \mathrm{~h}$ in eutrophic pond or eutrophic lake, and $\mathrm{t}_{1 / 2}=1.5 \mathrm{~h}$ in oligotrophic lake (Smith et al. 1978; quoted, Harris 1982)
$\mathrm{k}=2.8 \times 10^{-4} \mathrm{~s}^{-1}$ with $\mathrm{t}_{1 / 2}=1-2 \mathrm{~h}$ (Callahan et al., 1979)
calculated direct photolysis $\mathrm{k}=3.86 \times 10^{-4} \mathrm{~s}^{-1}$ in late January with $\mathrm{t}_{1 / 2}=0.69 \mathrm{~h}$ in pure water at 366 nm and in sunlight at $23-28^{\circ} \mathrm{C}$ and $\mathrm{k}=1.05 \times 10^{-5} \mathrm{~s}^{-1}$ in mid-December with $\mathrm{t}_{1 / 2}=1.1 \mathrm{~h}$ at 313 nm with $1-20 \%$ acetonitrile as cosolvent in filter-sterilized natural water (Mill et al. 1981)
$\mathrm{t}_{1 / 2}=0.37-1.1 \mathrm{~h}$, based on estimated photolysis half-life in air (Howard et al. 1991)
sunlight photolysis $\mathrm{t}_{1 / 2}=0.045 \mathrm{~d}$ for mid-December (Mill \& Mabey 1985)
half-lives on different atmospheric particulate substrates (approx. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=4.7 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=1.4 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=31 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985)
ozonation rate constant $\mathrm{k}<6.1 \times 10^{-4} \mathrm{~m} / \mathrm{s}$ was measured at $24^{\circ} \mathrm{C}$ with $\left[\mathrm{O}_{3}\right]=0.16 \mathrm{ppm}$ and light intensity of $1.3 \mathrm{~kW} / \mathrm{m}^{2}$ (Cope \& Kalkwarf 1987)
first order daytime decay $\mathrm{k}=0.0090 \mathrm{~min}^{-1}$ for soot particles loading of $1000-2000 \mathrm{ng} / \mathrm{mg}$ and $\mathrm{k}=0.0211$ $\mathrm{min}^{-1}$ with $30-350 \mathrm{ng} / \mathrm{mg}$ loading (Kamens et al. 1988)
photodegradation half-life was found ranging from 1 h in summer to days in winter (Valerio et al. 1991)
photodegradation $\mathrm{k}=0.0322 \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=0.35 \mathrm{~h}$ in ethanol-water ( $3: 7, \mathrm{v} / \mathrm{v}$ ) solution for initial concentration of 2.5 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
pseudo-first-order direct photolysis $\mathrm{k}($ exptl $)=0.0322 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=0.35 \mathrm{~h}$ and the predicted $\mathrm{t}_{1 / 2}=0.0416 \mathrm{~min}^{-1}$ calculated by QSPR method, in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{obs})=0.50 \mathrm{~h}, \mathrm{t}_{1 / 2}(\mathrm{calc})=0.57 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)
photochemical degradation under atmospheric conditions: $\mathrm{k}=(1.18 \pm 0.50) \times 10^{-4} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(1.63 \pm 0.48) \mathrm{h}$ in diesel particulate matter, rate constant $\mathrm{k}=(3.09 \pm 0.23) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(6.22 \pm 0.51) \mathrm{h}$ in diesel particulate matter/soil mixture, and $\mathrm{t}_{1 / 2}=0.35$ to 1.62 h in various soil components using a $900-\mathrm{W}$ photoirradiator as light source; rate constant $\mathrm{k}=(2.92 \pm 0.20) \times 10^{-5} \mathrm{~s}^{-1}$ and $\mathrm{t}_{1 / 2}=(6.59 \pm 0.49) \mathrm{h}$ in diesel particulate matter using a $300-\mathrm{W}$ light source (Matsuzawa et al. 2001)
Photodegradation $\mathrm{k}=2.1 \times 10^{-3} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Oxidation: rate constant k , for gas-phase second order rate constants, $\mathrm{k}_{\mathrm{OH}}$ for reaction with OH radical, $\mathrm{k}_{\mathrm{NO}_{3}}$ with $\mathrm{NO}_{3}$ radical and $\mathrm{k}_{\mathrm{O}_{3}}$ with $\mathrm{O}_{3}$ or as indicated, *data at other temperatures see reference:
$t_{1 / 2}>340 \mathrm{~h}$ in river water, eutrophic pond or lake and oligotrophic lake, half-lives predicted by one compartment model (Smith et al. 1978)
$\mathrm{k}($ aquatic fate rate $)=1680 \mathrm{M}^{-1} \mathrm{~s}^{-1}$, with half-life of 96 h (Callahan et al. 1979)
$\mathrm{t}_{1 / 2}=1500 \mathrm{~h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^{\circ} \mathrm{N}$, midday, midsummer (Zepp \& Schlotzhauer 1979)
$\mathrm{k}=5 \times 10^{8} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $2 \times 10^{4} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982)
$\mathrm{k}=0.62 \times 10^{4} \mathrm{dm}^{3} \mathrm{~mol}^{-1} \mathrm{~s}^{-1}$ for the reaction with $\mathrm{O}_{3}$ in water at pH 7 and $25^{\circ} \mathrm{C}$ with $\mathrm{t}_{1 / 2}=1.0 \mathrm{~s}$ in presence of $10^{-4} \mathrm{M}$ of ozone at pH 7 (Butković et al. 1983)
$\mathrm{k}(\mathrm{aq})=.3.6 \times 10^{-4} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=0.5 \mathrm{~h}$ under natural sunlight conditions; $\mathrm{k}(\mathrm{aq})=.1.9 \times 10^{3} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=4.3 \mathrm{~d}$ free-radicals oxidation in air-saturated water (NRCC 1983)
photooxidation $\mathrm{t}_{1 / 2}=0.428-4.28 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)
$\mathrm{k}_{\mathrm{HO}}$ (calc) $=1 \times 10^{10} \mathrm{M}^{-1} \mathrm{~s}^{-1}$ with hydroxyl radical in aqueous solutions (Haag \& Yao 1992)
Hydrolysis: not hydrolyzable (Mabey et al. 1982; Howard et al. 1991).
Biodegradation:
$\mathrm{t}_{1 / 2}>10000 \mathrm{~h}$ (quoted, Smith et al. 1978)
$\mathrm{k}=0.2-0.9 \mu_{\mathrm{mol}^{-1} \mathrm{mg}^{-1}}$ for bacterial protein (Callahan et al. 1979)
$\mathrm{k}=3.4 \times 10^{-4} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}=83 \mathrm{~h}$ for mixed bacterial populations in stream sediment (NRCC 1983)
$\mathrm{k}<3 \times 10^{-5} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}>2.5 \mathrm{yr} ; \mathrm{k}<3.0 \times 10^{-5} \mathrm{~h}^{-1}$ with $\mathrm{t}_{1 / 2}>2.5 \mathrm{yr}$ for mixed bacterial populations in oilcontaminated and pristine stream sediments (NRCC 1983)
$\mathrm{k}=3.5 \times 10^{-5} \mathrm{~h}^{-1}$ estimated in water and soil (Ryan \& Cohen 1986)
$\mathrm{t}_{1 / 2}($ aq. aerobic $)=57 \mathrm{~d}$ to 1.45 yr at $10-30^{\circ} \mathrm{C}$, soil die-away test (Coover \& Sims 1987; quoted, Howard et al. 1991); $\mathrm{k}=0.0022 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=309 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0030 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=229 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990)
$\mathrm{t}_{1 / 2}($ aq. anaerobic $)=228 \mathrm{~d}$ to 5.8 yr , based on estimated unacclimated aqueous aerobic biodegradation halflife (Coover \& Sims 1987; quoted, Howard et al. 1991).
Biotransformation: estimated to be $3 \times 10^{-12} \mathrm{~mL} \mathrm{cell}^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=49 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.010 \mathrm{~h}^{-1}$ (bluegill sunfish, Spacie et al. 1983)
$\mathrm{k}_{1}=131.1 \mathrm{~mL} \mathrm{~g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0033 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, $P$. hoyi, Landrum 1988)
$\mathrm{k}_{1}=81.3 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.014 \mathrm{~h}^{-1}$ (10-20 ${ }^{\circ} \mathrm{C}$, H. limbata, Landrum \& Poore 1988)
$\mathrm{k}_{1}=16.8 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0016 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, P. hoyi, Landrum \& Poore 1988)
$\mathrm{k}_{1}=87.8 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.012 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, S. heringianus, quoted, Landrum \& Poore 1988)
$\mathrm{k}_{1}=112.0 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.013 \mathrm{~h}^{-1}\left(4^{\circ} \mathrm{C}\right.$, Mysis relicta, quoted, Landrum \& Poore 1988)
$\mathrm{k}_{1}=75.9 \mathrm{~mL} \mathrm{~g}^{-1} \mathrm{~h}^{-1}$ (Pontoporeia hoyi, Evans \& Landrum 1989)
$\mathrm{k}_{1}=39.9 \mathrm{~mL} \mathrm{~g}^{-1} \mathrm{~h}^{-1}$ (Mysis relicta, Evans \& Landrum 1989)
$\mathrm{k}_{2}=0.0017 \mathrm{~h}^{-1}$ (Amphipods, Evans \& Landrum 1989)
$\mathrm{k}_{2}=0.0047 \mathrm{~h}^{-1}$ (Mysids, Evans \& Landrum 1989)
$\mathrm{k}_{1}=0.11-0.36 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0032 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.37-1.1 \mathrm{~h}$, based on estimated photolysis half-life (Lyman et al. 1982; quoted, Howard et al. 1991); half-lives under simulated atmospheric conditions: $\mathrm{t}_{1 / 2}=5.30 \mathrm{~h}$ in simulated sunlight, $\mathrm{t}_{1 / 2}=0.58 \mathrm{~h}$ in simulated sunlight + ozone ( 0.2 ppm ), $\mathrm{t}_{1 / 2}=0.62 \mathrm{~h}$ in dark reaction ozone ( 0.2 ppm ) (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983);
$\mathrm{t}_{1 / 2}=14 \mathrm{~h}$ with a steady-state concn of tropospheric ozone of $2 \times 10^{-9} \mathrm{M}$ in clean air (Butković et al. 1983);
photooxidation $t_{1 / 2}=0.428-4.28 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}=0.5 \mathrm{~h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated $\mathrm{k}=0.0234 \mathrm{~min}^{-1}$ at $1 \mathrm{cal} \mathrm{cm}^{-2} \mathrm{~min}^{-1}, 10 \mathrm{~g} \mathrm{~m}^{-3} \mathrm{H}_{2} \mathrm{O}$ and $20^{\circ} \mathrm{C}$ (Kamens et al. 1988).
Surface Water: $\mathrm{t}_{1 / 2}=2 \mathrm{~h}$ in methanol solution irradiated at 254 nm (Lu et al. 1977);
half-lives predicted by one compartment model: $\mathrm{t}_{1 / 2}>340 \mathrm{~h}$ in river water, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
very slow, not an important process (Callahan et al. 1979);
computed near-surface half-life for direct photochemical transformation of a natural water body $\mathrm{t}_{1 / 2}=0.54$ h at latitude $40^{\circ} \mathrm{N}$, midday, midsummer, and direct photolysis, $\mathrm{t}_{1 / 2}=3.2 \mathrm{~d}$ (no sediment-water partitioning) and $\mathrm{t}_{1 / 2}=13 \mathrm{~d}$ (with sediment-water partitioning) in a $5-\mathrm{m}$ deep inland water body (Zepp \& Schlotzhauer 1979);
$\mathrm{t}_{1 / 2}=0.37-1.1 \mathrm{~h}$, based on photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}=1.0 \mathrm{~s}$ in presence of $10^{-4} \mathrm{M}$ of ozone at pH 7 (Butković et al. 1983);
$\mathrm{t}_{1 / 2}=4.3 \mathrm{~d}$ free-radical oxidation in air-saturated water (NRCC 1983);
$t_{1 / 2}=0.045 \mathrm{~d}$ under mid-December sunlight (Mill \& Mabey 1985);
photolysis $\mathrm{t}_{1 / 2}=0.35 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater: $\mathrm{t}_{1 / 2}=2736-25440 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment: uptake clearance from sediment $\mathrm{k}=(0.0023 \pm 0.001) \mathrm{g}$ of dry sediment $\cdot \mathrm{g}^{-1}$ of organism $\cdot \mathrm{h}^{-1}$ for amphipod, $P$. hoyi in Lake Michigan sediments at $4^{\circ} \mathrm{C}$ (Landrum 1989);
desorption $\mathrm{t}_{1 / 2}=19.5 \mathrm{~d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: $t_{1 / 2}>2$ d (Sims \& Overcash 1983; quoted, Bulman et al. 1987);
$\mathrm{t}_{1 / 2}=347 \mathrm{~d}$ for $5 \mathrm{mg} / \mathrm{kg}$ treatment and $\mathrm{t}_{1 / 2}=218 \mathrm{~d}$ for $50 \mathrm{mg} / \mathrm{kg}$ treatment (Bulman et al. 1987);
biodegradation $\mathrm{k}=0.002 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=309 \mathrm{~d}$ for Kidman sandy loam soils and $\mathrm{k}=0.0030 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=229$ d for Mclaurin sandy loam soils (Park et al. 1990);
$t_{1 / 2}=1368-12720 \mathrm{~h}$, based on aerobic soil dieaway test data at $10-30^{\circ} \mathrm{C}$ (Groenewegen \& Stolp 1976; Coover \& Sims 1987; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
$\mathrm{t}_{1 / 2}=0.3$ to $>300 \mathrm{wk}, 8.2 \mathrm{yr}$ (literature, Luddington soil, Wild et al. 1991).
Biota: depuration $t_{1 / 2}=18 \mathrm{~d}$ by oysters (Lee et al. 1978; quoted, Verschueren 1983);
$\mathrm{t}_{1 / 2}=67 \mathrm{~h}$ in bluegill sunfish (Spacie et al. 1983);
depuration $\mathrm{t}_{1 / 2}=52 \mathrm{~h}$ in $s$. heringianus (Frank et al. 1986);
calculated half-lives in different tissues of sea bass: $\mathrm{t}_{1 / 2}=12.4 \mathrm{~d}$ for fat, $\mathrm{t}_{1 / 2}=6.5 \mathrm{~d}$ for kidney, $\mathrm{t}_{1 / 2}=5.1 \mathrm{~d}$ for kidney, $\mathrm{t}_{1 / 2}=5.1 \mathrm{~d}$ for intestine, $\mathrm{t}_{1 / 2}=4.8 \mathrm{~d}$ for gallbladder, $\mathrm{t}_{1 / 2}=4.5 \mathrm{~d}$ for spleen, $\mathrm{t}_{1 / 2}=2.9 \mathrm{~d}$ for muscle, $\mathrm{t}_{1 / 2}=2.4 \mathrm{~d}$ for whole body, $\mathrm{t}_{1 / 2}=2.3 \mathrm{~d}$ for gonads, $\mathrm{t}_{1 / 2}=2.3 \mathrm{~d}$ for gills, and $\mathrm{t}_{1 / 2}=2.2 \mathrm{~d}$ for liver (Lemaire et al. 1990);
elimination $\mathrm{t}_{1 / 2}=4.8-16 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=7 \mathrm{~d}$ from polychaete Abarenicola pacifica, $\mathrm{t}_{1 / 2}=$ 21.7 d from Oyster, $\mathrm{t}_{1 / 2}=8.0 \mathrm{~d}$ from clam Mercenario mercenaria, $\mathrm{t}_{1 / 2}=8 \mathrm{~d}$ from clam Rangia cuneata (quoted, Meador et al. 1995);
$\mathrm{t}_{1 / 2}=15-17 \mathrm{~d}$ for blue mussel Mytilus edulis in 32-d exposure laboratory studies (Magnusson et al. 2000).

TABLE 4.1.1.43.1
Reported aqueous solubilities and Henry's law constants of benzo[a]pyrene at various temperatures

$$
\begin{equation*}
\ln x=\mathrm{A}+\mathrm{B} /(\mathrm{T} / \mathrm{K})+\mathrm{C} \cdot \ln (\mathrm{~T} / \mathrm{K}) \tag{1}
\end{equation*}
$$

Aqueous solubility

| Aqueous solubility |  |  |  |  |  | Henry's law constant |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| May et al. 1983 |  | Velapoldi et al. 1983 |  | Whitehouse 1984 |  | ten Hulscher et al. 1992 |  |
| generator column-HPLC |  | generator column-fluorescence |  | generator column-HPLC |  | gas strippingHPLC/fluorescence |  |
| $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t /{ }^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $t^{\circ} \mathrm{C}$ | $\mathrm{S} / \mathrm{g} \cdot \mathrm{m}^{-3}$ | $\mathrm{t}^{\circ} \mathrm{C}$ | Pa m ${ }^{3} / \mathrm{mol}$ |
| 10 | 0.00056 | 10 | 0.00061 | 8.0 | 0.00066 | 10.0 | 0.022 |
| 15 | 0.00080 | 15 | 0.00082 | 12.4 | 0.00077 | 20.0 | 0.034 |
| 20 | 0.00114 | 20 | 0.00113 | 16.7 | 0.00094 | 35.0 | 0.074 |
| 25 | 0.00162 | 25 | 0.00158 | 20.9 | 0.00116 | 40.1 | 0.092 |
| 30 | 0.00229 | 30 | 0.00224 | 25.0 | 0.00154 | 45.0 | 0.110 |
|  |  |  |  |  |  | 55.0 | 0.239 |
|  |  | eq. 1 | x |  |  |  |  |
|  |  | A | -677.4109 |  |  | $\begin{aligned} & \ln \mathrm{K}_{\mathrm{AW}}=-\Delta \mathrm{H} / \mathrm{RT}+\Delta \mathrm{S} / \mathrm{R} \\ & \mathrm{R}=8.314 \mathrm{~Pa} \mathrm{~m}^{3} \mathrm{~mol}^{-1} \mathrm{~K}^{-1} \end{aligned}$ |  |
|  |  | B | 23963.0 |  |  |  |  |
|  |  | C | 100.767 |  |  | $\Delta \mathrm{S} / \mathrm{R}$ | 11.90 |
|  |  |  |  |  |  | $\Delta \mathrm{H} / \mathrm{R}$ | 4690.88 |
|  |  | $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=50.6$ |  |  |  | enthalpy of volatilization: <br> $\Delta \mathrm{H} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=39 \pm 3$ |  |
|  |  |  | at $25^{\circ} \mathrm{C}$ |  |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  | entropy of volatilization, $\Delta \mathrm{S}$ |  |
|  |  |  |  |  |  | $\mathrm{T} \Delta \mathrm{S} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=29 \pm 3$ |  |
|  |  |  |  |  |  | at $20^{\circ} \mathrm{C}$ |  |



FIGURE 4.1.1.43.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for benzo[a]pyrene.

### 4.1.1.44 Benzo[e]pyrene



Common Name: Benzo[e]pyrene
Synonym: B [e]P, 4,5-benzopyrene
Chemical Name: 4,5-benzopyrene
CAS Registry No: 192-97-2
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{12}$
Molecular Weight: 252.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
181.4 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 311 (Lide 2003)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
222.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999)
262.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 16.57 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
42.30 (differential scanning calorimetry, Hinckley et al. 1990)
36.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0292\left(\mathrm{mp}\right.$ at $181.4^{\circ} \mathrm{C}$ ) 0.010 (calculated, Passivirta et al. 1999)

Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.0035 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.00732 (shake flask-UV/fluorescence, Barone et al. 1967)
$0.00014,0.000172,0.0000252$ (HPLC-relative retention correlation, different stationary and phases, Locke 1974)
$0.0050^{*} \quad\left(23^{\circ} \mathrm{C}\right.$, shake flask-fluorescence, measured range $8.6-31.7^{\circ} \mathrm{C}$, Schwarz 1977)
$0.00732,0.004 ; 0.0063$ (quoted values; lit. mean, Pearlman et al. 1984)
$\log \mathrm{S}_{\mathrm{L}}(\mathrm{mol} / \mathrm{L})=-1.398-866.8 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$\ln x=-11.8754-2916.84 /(\mathrm{T} / \mathrm{K})$; temp range $5-50^{\circ} \mathrm{C}$ (regression eq. of literature data, Shiu \& Ma 2000)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$7.40 \times 10^{-7}$ (Knudsen effusion method, extrapolated, Murray et al. 1974)
$\log (\mathrm{P} / \mathrm{mmHg})=9.736-6220 /(\mathrm{T} / \mathrm{K})$; temp range $359-423 \mathrm{~K}$ (Knudsen effusion method, Murray et al. 1974) $7.58 \times 10^{-7}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.7417-6220 /(\mathrm{T} / \mathrm{K})$; temp range $358-423 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987) $3.20 \times 10^{-7}, 1.28 \times 10^{-5}\left(20^{\circ} \mathrm{C}\right.$, literature solid $\mathrm{P}_{\mathrm{S}}$, converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with $\Delta \mathrm{S}_{\text {fus }}$ Bidleman \& Foreman 1987)
$8.59 \times 10^{-5}\left(\mathrm{P}_{\mathrm{GC}}\right.$, GC-RT correlation with $p, p=-\mathrm{DDT}$ as reference standard, Hinckley et al. 1990)
$2.53 \times 10^{-5}, 1.02 \times 10^{-5}$ (supercooled liquid values $\mathrm{P}_{\mathrm{L}}$, converted from literature $\mathrm{P}_{\mathrm{S}}$ with different $\Delta \mathrm{S}_{\text {fus }}$ values, Hinckley et al. 1990)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=11.11-4803 /(\mathrm{T} / \mathrm{K})(\mathrm{GC}-\mathrm{RT}$ correlation, Hinckley et al. 1990)
$1.29 \times 10^{-5}$ (supercooled liquid values $P_{L}$, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
$1.78 \times 10^{-5} ; 1.78 \times 10^{-6}$ (quoted supercooled liquid $\mathrm{P}_{\mathrm{L}}$ from Hinckley et al. 1990; converted to solid $\mathrm{P}_{\mathrm{S}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.15-5333 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=10.14-4467 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
0.02 (calculated-P/C, Mackay et al. 1992)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=11.64-3660 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ :
6.44 (calculated-MCI $\chi$ as per Rekker \& De Kort 1979, Ruepert et al. 1985)
7.40 (calculated- $\mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)
6.44 (TLC retention time correlation, De Voogt et al. 1990)
6.44 (recommended, Sangster 1993)
6.10 (quoted, Meador et al. 1995)
5.68 (calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
11.13 (calculated, Finizio et al. 1997)

Bioconcentration Factor, $\log \mathrm{BCF}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
7.20
4.00
6.11-7.90; 7.20-8.30
$5.84 ; 6.12,6.11,6.62$
(Baltic Sea particulate field samples, conen distribution-GC/MS, Broman et al. 1991) (predicted dissolved $\log \mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)
(range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$20^{\circ} \mathrm{C}$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants or Half-Lives:
Bioconcentration, Uptake $\left(\mathrm{k}_{1}\right)$ and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:
$\mathrm{k}_{1}=0.13-0.36 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0031 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:
Air: half-lives under simulated atmospheric conditions: $\mathrm{t}_{1 / 2}=21.10 \mathrm{~h}$ in simulated sunlight, $\mathrm{t}_{1 / 2}=5.38 \mathrm{~h}$ in simulated sunlight + ozone ( 0.2 ppm ), $\mathrm{t}_{1 / 2}=7.6 \mathrm{~h}$ in dark reaction ozone ( 0.2 ppm ) (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $\mathrm{t}_{1 / 2}=6.9-14.4 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=30.1 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=4.7 \mathrm{~d}$ from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.44.1
Reported aqueous solubilities of benzo[e]pyrene at various temperatures
Schwarz 1977

| shake flask-fluorescence |  |
| ---: | ---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |
| 8.6 | $3.25 \times 10^{-3}$ |
| 14.0 | $3.58 \times 10^{-3}$ |
| 17.0 | $4.44 \times 10^{-3}$ |
| 17.5 | $3.94 \times 10^{-3}$ |

TABLE 4.1.1.44.1 (Continued)
Schwarz 1977

| shake flask-fluorescence |  |  |  |
| :--- | ---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{S} / \mathbf{g} \cdot \mathbf{m}^{-3}$ |  |  |
| 20.2 | $4.79 \times 10^{-3}$ |  |  |
| 23.2 | $5.35 \times 10^{-3}$ |  |  |
| 23.0 | $5.07 \times 10^{-3}$ |  |  |
| 29.2 | $6.38 \times 10^{-3}$ |  |  |
| 29.2 | $6.48 \times 10^{-3}$ |  |  |
| 31.7 | $6.81 \times 10^{-3}$ |  |  |
| $\Delta \mathrm{H}_{\text {sol }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=25.56$ |  |  |  |
|  |  |  |  |

### 4.1.1.45 Perylene



Common Name: Perylene
Synonym: peri-dinaphthalene
Chemical Name: perylene
CAS Registry No: 198-55-0
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{12}$
Molecular Weight: 252.309
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
277.76 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
503 (Pearlman et al. 1984)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $25^{\circ} \mathrm{C}$ ): 1.35 (Lide 2003)

Molar Volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ : $186.9 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
222.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999)
262.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
23.51 (quoted, Tsonopoulos \& Prausnitz 1971)
31.753 (Ruelle \& Kesselring 1997)
31.88 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
42.68 (quoted, Tsonopoulos \& Prausnitz 1971)
57.4 (Passivirta et al. 1999)
67.87, 43.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.00331\left(\mathrm{mp}\right.$ at $277.76^{\circ} \mathrm{C}$ ) 0.00268 (calculated, Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$0.0005 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry Davis et al. 1942)
$<0.0005$ (Weimer \& Prausnitz 1965)
$0.00011 \quad\left(20^{\circ} \mathrm{C}\right.$, shake flask-UV, Eisenbrand \& Baumann 1970)
0.0004 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.0003 (average lit. value, Pearlman et al. 1984)
0.0007 (microdroplet sampling and multiphoton ionization-based fast-conductivity technique MPI-FC, Gridin et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-0.306-1662 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$\log (\mathrm{P} / \mathrm{mmHg})=13.95-7260 /(\mathrm{T} / \mathrm{K})$; temp range $110-180^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958) $5.31 \times 10^{-9}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=13.075-7260 /(\mathrm{T} / \mathrm{K})$; temp range $383-453 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.9379-7210 /(\mathrm{T} / \mathrm{K})$; temp range $383-516 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987) $7.00 \times 10^{-7} \quad$ (quoted, Riederer 1990)
$1.84 \times 10^{-8 *}$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $118-210^{\circ} \mathrm{C}, \mathrm{Oja}$ \& Suuberg 1998)
$\ln (\mathrm{P} / \mathrm{Pa})=35.702-15955 /(\mathrm{T} / \mathrm{K})$; temp range $391-424 \mathrm{~K}$ (Clausius-Clapeyron eq., Knudsen effusion, Oja \& Suuberg 1998)
$1.40 \times 10^{-8} ; 5.22 \times 10^{-6}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.53-6074 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.53-4414 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$4.88 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4694 /(\mathrm{T} / \mathrm{K})+10.43 ; \Delta \mathrm{H}_{\text {vap }} .=-89.9 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ and the report temperature dependence equations):
0.440 (calculated-P/C, Riederer 1990)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=9.84-2752 /(\mathrm{T} / \mathrm{K})$, (Passivirta et al. 1999)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
6.30, 5.10 (HPLC-RV predicted, Brooke et al. 1986)
5.30 (HPLC-RV measured, Brooke et al. 1986)
5.82 (HPLC-RT correlation, Wang et al. 1986)
6.25 (recommended, Sangster 1989, 1994)
6.40 (Bayona et al. 1991)
5.82 (recommended, Hansch et al. 1995)
6.50 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson \& Schrăder 1999)
6.25; 6.53 (quoted lit.; calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :

Bioconcentration Factor, $\log \mathrm{BCF}$ :

| $3.86,3.73$ | (Daphnia pulex, kinetic estimation, Southworth et al. 1978) <br> 4.36 <br> $3.30,4.36,<1.0$ |
| :--- | :--- |
| (activated sludge, Freitag et al. 1984)  <br> 3.85 (algae, activated sludge, fish, Klein et al. 1984) <br> $3.30,4.36,<1.0$ (Daphnia pulex, correlated as per Mackay \& Hughes 1984, Hawker \& Connell 1986) <br> 3.86 (algae, activated sludge, fish, Freitag et al. 1985) <br> $1.196,-0.398$ (Daphnia magna, Newsted \& Giesy 1987) <br> (Polychaete sp, Capitella capitata, Bayona et al. 1991)  |  |

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
6.39-7.93 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$5.88 ; 6.73,6.63,6.76\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)
6.30; 5.89; 4.15-6.38 (calculated- $\mathrm{K}_{\text {Ow }}$; calculated-solubility; quoted lit. range, Schlautman \& Morgan 1993a) 6.05 at $\mathrm{pH} 4,5.98$ at $\mathrm{pH} 7,5.71$ at pH 10 in $0.001 \mathrm{M} \mathrm{NaCl} ; 6.01$ at $\mathrm{pH} 4,5.95$ at $\mathrm{pH} 7,5.29$ at pH 10 in 0.01 $\mathrm{M} \mathrm{NaCl} ; 5.98$ at $\mathrm{pH} 4,5.67$ at $\mathrm{pH} 7,4.86$ at pH 10 in $0.1 \mathrm{M} \mathrm{NaCl} ; 5.97$ at $\mathrm{pH} 4,5.61$ at $\mathrm{pH} 7,4.78$ at pH 10 in $1 \mathrm{mMCa}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substanceshumic acid; Schlautmam \& Morgan 1993)
5.17 at pH 4 in $0.001 \mathrm{M} \mathrm{NaCl} ; 5.14$ at pH 4 in $0.01 \mathrm{M} \mathrm{NaCl} ; 5.08$ at pH 4 in $0.1 \mathrm{M} \mathrm{NaCl} ; 5.11$ at pH 4 in $1 \mathrm{mM} \mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substancesfulvic acid; Schlautmam \& Morgan 1993a, b)
5.82 at $\mathrm{pH} 4,<4.49$ at $\mathrm{pH} 7,<4.18$ at pH 10 in $0.001 \mathrm{M} \mathrm{NaCl} ; 5.65$ at $\mathrm{pH} 4,<4.46$ at $\mathrm{pH} 7,<3.85$ at pH 10 in $0.01 \mathrm{M} \mathrm{NaCl} ; 5.67$ at $\mathrm{pH} 4,<4.17$ at $\mathrm{pH} 7,<3.78$ at pH 10 in $0.1 \mathrm{M} \mathrm{NaCl} ; 5.74$ at $\mathrm{pH} 4,5.02$ at pH 7 , 4.43 at pH 10 in $1 \mathrm{mM} \mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-humic acid; Schlautmam \& Morgan 1993b)
$<3.48$ at pH 4 in $0.001 \mathrm{M} \mathrm{NaCl} ;<3.30$ at pH 4 in $0.01 \mathrm{M} \mathrm{NaCl} ;<3.48$ at pH 4 in $0.1 \mathrm{M} \mathrm{NaCl} ;<3.48$ at pH 4 in $1 \mathrm{mM} \mathrm{Ca}^{2+}$ in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substancesfulvic acid; Schlautmam \& Morgan 1993b)
6.00 (soil humic acid, shake flask-HPLC/UV, Cho et al. 2002)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization: sublimation $\mathrm{k}<1 \times 10^{-5} \mathrm{~s}^{-1}$ from glass surface was measured at $24^{\circ} \mathrm{C}$ at an airflow rate of $3 \mathrm{~L} / \mathrm{min}$ (Cope \& Kalkwarf 1987).
Photolysis:
half-lives on different atmospheric particulate substrates (appr. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=3.9 \mathrm{~h}$ on silica gel, $\mathrm{t}_{1 / 2}=1.2 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=35 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985)
ozonation $\mathrm{k}<4.7 \times 10^{-5} \mathrm{~m} / \mathrm{s}$ was measured from glass surface at $24^{\circ} \mathrm{C}$ with $\left[\mathrm{O}_{3}\right]=0.16 \mathrm{ppm}$ and light intensity of $1.3 \mathrm{~kW} / \mathrm{m}^{2}$ (Cope \& Kalkwarf 1987)
photodegradation $\mathrm{k}=0.0152 \mathrm{~min}^{-1}$ and $\mathrm{t}_{1 / 2}=0.78 \mathrm{~h}$ in ethanol-water $(2: 3, \mathrm{v} / \mathrm{v})$ solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
$\mathrm{k}(\operatorname{expt})=0.0152 \mathrm{~min}^{-1}$ the pseudo-first-order rate constant with the calculated $\mathrm{t}_{1 / 2}=0.78 \mathrm{~h}$ and the predicted $\mathrm{k}=0.0406 \mathrm{~min}^{-1}$, calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);
$\mathrm{t}_{1 / 2}=0.53 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)
Photodegradation $\mathrm{k}=4.4 \times 10^{-4} \mathrm{~s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht \& Blough 2002)
Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=752 \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.139 \mathrm{~h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)
$\log \mathrm{k}_{1}=2.88 \mathrm{~h}^{-1} ; \log \mathrm{k}_{2}=-0.86 \mathrm{~h}^{-1}$ (Daphnia pulex, correlated as per Mackay \& Hughes 1984, Hawker \& Connell 1986)
$\mathrm{k}_{1}=0.12-0.38 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0034 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:
Air: direct photolysis $t_{1 / 2}=0.53 \mathrm{~h}$ (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).
Surface water: photolysis $t_{1 / 2}=0.78 \mathrm{~h}$ (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: elimination half-lives: $\mathrm{t}_{1 / 2}=2.0$ d from rainbow trout, $\mathrm{t}_{1 / 2}=26.2 \mathrm{~d}$ from clam Mya arenaria, $\mathrm{t}_{1 / 2}=6.3-13.3 \mathrm{~d}$ from mussel Mytilus edulis; $\mathrm{t}_{1 / 2}=9.2 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=1.2 \mathrm{~d}$ from shrimp, $\mathrm{t}_{1 / 2}=5.7 \mathrm{~d}$ from polychaete Nereis virens, $\mathrm{t}_{1 / 2}=8.0$ d from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.45.1
Reported vapor pressures of perylene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- |
| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}$ | $=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ |  |

$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$

Hoyer \& Peperle $1958 \quad$ Oja \& Suuberg 1998

| effusion | Knudsen effusion |  |
| :---: | :---: | :---: |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | t/ ${ }^{\circ} \mathrm{C}$ | P/Pa |
| data presented by equation | 124.10 | 0.0114 |
| eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | 127.37 | 0.0164 |
| A 13.95 | 131.82 | 0.0249 |
| B 7260 | 135.96 | 0.0373 |

TABLE 4.1.1.45.1 (Continued)

| Hoyer \& Peperle 1958 | Oja \& Suuberg 1998 |
| :---: | :---: |
| effusion | Knudsen effusion |
| $\mathbf{t /}{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathrm{Pa}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ |
| for temp range $110-180^{\circ} \mathrm{C}$ | 141.870 .0638 |
| $\mathrm{mp} /{ }^{\circ} \mathrm{C} \quad 270.5-273.5$ | mp/K 551 |
| $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ} / \mathrm{mol})=140.1$ | eq. 1a $\mathrm{P} / \mathrm{Pa}$ |
|  | A $\quad 35.702$ |
|  | B 15955 |
|  | for temp range 391-424 K |
|  | $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJJ} / \mathrm{mol})=132.6$ |



FIGURE 4.1.1.45.1 Logarithm of vapor pressure versus reciprocal temperature for perylene.

### 4.1.1.46

## 7,12-Dimethylbenz[a]anthracene



Common Name: 7,12-Dimethylbenz[a]anthracene
Synonym: 7,12-dimethylbenz[a]anthracene, 9,10-dimethyl-1,2-benzanthracene, 7,12-dimethylbenzanthracene
Chemical Name: 7,12-dimethylbenz[a]anthracene
CAS Registry No: 57-97-6
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{16}$
Molecular Weight: 256.341
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
122.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$245.8 \quad$ (Ruelle \& Kesselring 1997)
292.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})$ : $104.56 \quad($ Kelley \& Rice 1964)
Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 22.09 (Kelley \& Rice 1964)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}$ ( $\mathrm{J} / \mathrm{mol} \mathrm{K):}$
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.111 ( mp at $122.5^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$0.043 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.061 (shake flask-fluorescence, Mackay \& Shiu 1977)
$0.053 \quad\left(24^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Hollifield 1979)
$0.025 \quad\left(24^{\circ} \mathrm{C}\right.$, shake flask-LSC, Means et al. 1979)
0.0244 (shake flask-LSC, Means et al. 1980b)
$0.043,0.061,0.053 ; 0.054$ (quoted lit. values; lit. mean, Pearlman et al. 1984)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
$3.73 \times 10^{-7}$ (solid vapor pressure, extrapolated, effusion method, Kelley \& Rice 1974)
$3.70 \times 10^{-6}$ (extrapolated, supercooled liquid value $\mathrm{P}_{\mathrm{L}}$, Kelley \& Rice 1974)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{mmHg}\right)=15.108-7051 /(\mathrm{T} / \mathrm{K})$; temp range: $106-122^{\circ} \mathrm{C}$ (effusion method, Kelley \& Rice 1964)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{mmHg}\right)=12.232-5987 /(\mathrm{T} / \mathrm{K})$; temp range: $122-135^{\circ} \mathrm{C}$ (effusion method, Kelley \& Rice 1964)
$3.84 \times 10^{-7}$ (extrapolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=14.233-7051 /(\mathrm{T} / \mathrm{K})$; temp range $379-396 \mathrm{~K}$ (Antoine eq.-I, Stephenson \& Malanowski 1987)
$6.78 \times 10^{-6}$ (extrapolated-Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.70417-5629.911 /(\mathrm{T} / \mathrm{K})$; temp range $379-390 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=11.357-5897 /(\mathrm{T} / \mathrm{K})$, temp range $396-408 \mathrm{~K}$ (Antoine eq.-III, Stephenson \& Malanowski 1987) $6.38 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4643 /(\mathrm{T} / \mathrm{K})+10.38 ; \Delta \mathrm{H}_{\text {vap }}=-88.9 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :
5.98 (shake flask-LSC, concn. ratio, Means et al. 1979)
5.80 (shake flask-LSC, Means et al. 1980b)
6.16 (UNIFAC activity coeff., Banerjee \& Howard 1988)
5.80 (recommended, Sangster 1989)
5.89 (recommended, Sangster 1993)
5.80 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
5.68 (average of 3 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1979)
5.37 (average of 12 soil/sediment samples, sorption isotherms by shake flask-LSC, Means et al. 1980b)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Hydrolysis: no hydrolyzable groups (Howard et al. 1991).
Oxidation: photooxidation $t_{1 / 2}=0.32-3.2 \mathrm{~h}$ estimated, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991); photooxidation $\mathrm{t}_{1 / 2}$ (aq.) $=1,57-157 \mathrm{yr}$ estimated, based on measured rate constant for the reaction with singlet oxygen in benzene (Stevens et al. 1974; quoted, Howard et al. 1991).
Biodegradation: biodegradation $\mathrm{k}=0.0339 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=20 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{k}=0.0252 \mathrm{~d}^{-1}$ with $t_{1 / 2}=28 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$\mathrm{t}_{1 / 2}$ (aq. aerobic) ~480-672 h, based on aerobic soil die-away test data (Sims 1990; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}$ (aq. anaerobic) ~ 1920-2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.32-3.2 \mathrm{~h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1 / 2}=480-672 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=960-1344 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: biodegradation rate constant $\mathrm{k}=0.0339 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=20 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{k}=0.0252 \mathrm{~d}^{-1}$ with $t_{1 / 2}=28 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990); $\mathrm{t}_{1 / 2} \sim 480-672 \mathrm{~h}$, based on aerobic soil die-away test data (Howard et al. 1991).

### 4.1.1.47 9,10-Dimethylbenz[a]anthracene



Common Name: 9,10-Dimethylbenz[a]anthracene
Synonym:
Chemical Name: 9,10-dimethylbenz[a]anthracene
CAS Registry No: 56-56-4
Molecular Formula: $\mathrm{C}_{20} \mathrm{H}_{16}$
Molecular Weight: 256.341
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
122 (Yalkowsky et al. 1983; Ruelle \& Kesselring 1997)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$245.8 \quad$ (Ruelle \& Kesselring 1997)
292.7 (calculated-Le Bas method at normal boiling point)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
54.81 (Kelley \& Rice 1974)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.112 ( mp at $122^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$0.0435 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.0435 (recommended, Shaw 1989)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equation):
$\log (\mathrm{P} / \mathrm{mmHg})=15.108-7051 /(\mathrm{T} / \mathrm{K})$; temp range: $106-135^{\circ} \mathrm{C}$ (effusion method, Kelley \& Rice 1964)
$\log (\mathrm{P} / \mathrm{mmHg})=12.232-5897 /(\mathrm{T} / \mathrm{K})$ (liquid, effusion method, Kelley \& Rice 1964)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
6.93 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 4.1.1.48 3-MethyIcholanthrene



Common Name: 3-Methylcholanthrene
Synonym: 20-methylcholanthrene, 1,2-dihydro-3-methyl-benz[j]aceanthrylene
Chemical Name: 3-methylcholanthrene
CAS Registry No: 56-49-5
Molecular Formula: $\mathrm{C}_{21} \mathrm{H}_{16}$
Molecular Weight: 268.352
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
180 (Bjørseth 1983)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ): 1.28 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 247.8 (Ruelle \& Kesselring 1997)
209.6 ( $20^{\circ} \mathrm{C}$, calculated-density)
296.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0301\left(\mathrm{mp}\right.$ at $180^{\circ} \mathrm{C}$ ) 0.003 (Mackay et al. 1980)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ ):
0.0015 (Weimer \& Prausnitz 1965)
0.0029 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.00323 (shake flask-liquid scintillation counting, Means et al. 1980)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations): $\log (\mathrm{P} / \mathrm{mmHg})=13.168-6643 /(\mathrm{T} / \mathrm{K})$; temp range $128-152^{\circ} \mathrm{C}$ (effusion method, Kelley \& Rice 1964) $1.03 \times 10^{-7}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987) $\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.293-6643 /(\mathrm{T} / \mathrm{K})$; temp range 401-425 K (Antoine eq., Stephenson \& Malanowski 1987) $1.48 \times 10^{-6}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4901 /(\mathrm{T} / \mathrm{K})+10.61 ; \Delta \mathrm{H}_{\text {vap }}=-93.8 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
6.42 (shake flask-LSC, Means et al. 1980)
7.11 (calculated-f const., Valvani \& Yalkowsky 1980)
6.69 (calculated-S and mp, Mackay et al. 1980)
7.11 (Hansch \& Leo 1985)
6.45, 7.07 (calculated-UNIFAC, calculated-fragment const., Banerjee \& Howard 1988)
$6.75 \pm 0.50$ (recommended, Sangster 1989)
6.45 (recommended, Sangster 1993)
6.42 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
4.12 (Daphnia magna, McCarthy et al. 1985)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
6.09 (soil/sediment, sorption isotherm by batch equilibrium-LSC, Means et al. 1980b)
6.25 (average of 14 soil/sediment samples, sorption isotherm by shake flask-LSC, Means et al. 1980)
6.09, 6.10 (calculated-regression of $\mathrm{K}_{\mathrm{p}}$ versus substrate properties, calculated.- $\mathrm{K}_{\mathrm{ow}}$, Means et al. 1980)
4.02 (soil, calculated- $\mathrm{K}_{\text {ow }}$, Briggs 1981)
6.18 (soil, calculated- $\mathrm{K}_{\mathrm{OW}}$, Means et al. 1982)
5.07 (soil, calculated-K ${ }_{\text {ow }}$, Chiou et al. 1983)

Environmental Fate Rate Constants, $k$ or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis:
Hydrolysis: no hydrolyzable groups (Howard et al. 1991).
Oxidation: photooxidation $\mathrm{t}_{1 / 2}=0.317-3.17 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Biodegradation: aerobic $\mathrm{t}_{1 / 2}=14616-33600 \mathrm{~h}$, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991);
anaerobic $\mathrm{t}_{1 / 2}=58464-134400 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life
(Howard et al. 1991).
Biotransformation:
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.317-3.17 \mathrm{~h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $\mathrm{t}_{1 / 2}=14616-33600 \mathrm{~h}$, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=29232-672000 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $\mathrm{t}_{1 / 2}=14616-33600 \mathrm{~h}$, based on estimated mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).
Biota:

### 4.1.1.49 Benzo[ghi]perylene



Common Name: Benzo[ghi]perylene
Synonym: 1,12-benzoperylene, benzoperylene
Chemical Name: 1,12-benzoperylene
CAS Registry No: 191-24-2
Molecular Formula: $\mathrm{C}_{22} \mathrm{H}_{12}$
Molecular Weight: 276.330
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): 272.5 (Lide 2003)

Boiling Point ( ${ }^{\circ} \mathrm{C}$ ): 525 (Pearlman et al. 1984)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
233.8 (Ruelle \& Kesselring 1997; Passivirta et al. 1999)
277.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
17.365 (Ruelle \& Kesselring 1997)
17.37 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 31.34, 43.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
31.4 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), $\mathrm{F}=0.00373\left(\mathrm{mp}\right.$ at $272.5^{\circ} \mathrm{C}$ )
0.039 (calculated, $\Delta \mathrm{S}_{\text {fus }}=31.4 \mathrm{~J} / \mathrm{mol} \mathrm{K}$, Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
0.00026 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.0007 (generator column-HPLC/fluo., Wise et al. 1981)
0.00083 (quoted, Pearlman et al. 1984)
0.000137 (generator column-HPLC/fluo., De Maagd et al. 1998)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-2.073-908.7 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations):
$1.39 \times 10^{-8}$ (Knudsen effusion method, Murray et al. 1974)
$\log (\mathrm{P} / \mathrm{atm})=9.519-6674 /(\mathrm{T} / \mathrm{K})$; temp range: 389-468 K (Knudsen effusion method, Murray et al. 1974)
$1.33 \times 10^{-8}\left(20^{\circ} \mathrm{C}\right.$, estimated, Callahan et al. 1979)
$6.69 \times 10^{-7}$ (Yamasaki et al. 1984)
$1.38 \times 10^{-8} ; 7.51 \times 10^{-9}$ (extrapolated-Antoine eq. I, II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.5247-6674 /(\mathrm{T} / \mathrm{K})$; temp range 389-468 K (Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=10.945-6580 /(\mathrm{T} / \mathrm{K})$; temp range $391-513 \mathrm{~K}$ (Antoine eq.-II, Stephenson \& Malanowski 1987)
$7.20 \times 10^{-6} ; 1.84 \times 10^{-6}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.40-5824 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=10.76-4915 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999) $4.28 \times 10^{-7}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-5018 /(\mathrm{T} / \mathrm{K})+10.46 ; \Delta \mathrm{H}_{\text {vap }}=-96.1 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.027^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, gas stripping-HPLC/fluorescence, measured range $10-55^{\circ} \mathrm{C}$, ten Hulscher et al. 1992)
$\log \left(\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right)=12.83-4006 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
$0.0278\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured values, Staudinger \& Roberts 1996 , 2001)
$\log \mathrm{K}_{\mathrm{AW}}=-0.651-1258 /(\mathrm{T} / \mathrm{K})$ (van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
7.10 (RP-TLC-k' correlation, Bruggeman et al. 1982)
7.05 (HPLC-RT correlation, Rapaport et al. 1984)
6.63 (HPLC-RT correlation, Wang et al. 1986)
6.90 (recommended, Sangster 1989, 1993)
7.04 (TLC retention time correlation, De Voogt et al. 1990)
6.63 (recommended, Hansch et al. 1995)
6.22 (range 5.95-6.38) (shake flask/slow stirring-HPLC/fluo., De Maagd et al. 1998)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
5.54 (microorganisms-water, calculated from $\mathrm{K}_{\mathrm{OW}}$, Mabey et al. 1982)
4.45 (Daphnia magna, Newsted \& Giesy 1987)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ at $25^{\circ} \mathrm{C}$ or as indicated:
6.70 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
$7.215\left(10^{\circ} \mathrm{C}\right), 7.08,6.93\left(20^{\circ} \mathrm{C}\right), 6.68\left(35^{\circ} \mathrm{C}\right), 6.46,6.51\left(45^{\circ} \mathrm{C}\right)\left(\log \mathrm{K}_{\mathrm{DOC}}\right.$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers \& ten Hulscher 1996)
$6.80 \quad\left(20^{\circ} \mathrm{C}, \log \mathrm{K}_{\mathrm{POC}}-\right.$ particulate organic material from lake, Lüers \& ten Hulscher 1996)
6.82-8.25; 6.20-9.20 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$5.87 ; 6.84,6.82,7.26\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: half-lives on different atmospheric particulate substrates (approx. $25 \mu \mathrm{~g} / \mathrm{g}$ on substrate): $\mathrm{t}_{1 / 2}=7.0 \mathrm{~h}$ on silica gel, $t_{1 / 2}=22 \mathrm{~h}$ on alumina and $\mathrm{t}_{1 / 2}=29 \mathrm{~h}$ on fly ash (Behymer \& Hites 1985);
first order daytime photodegradation rate constants for adsorption on wood soot particles in an outdoor Teflon chamber: $\mathrm{k}=0.0077 \mathrm{~min}^{-1}$ with $1000-2000 \mathrm{ng} / \mathrm{mg}$ loading and $\mathrm{k}=0.0116 \mathrm{~min}^{-1}$ with $30-350$ $\mathrm{ng} / \mathrm{mg}$ loading (Kamens et al. 1988);
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{obs})=0.89 \mathrm{~h}, \mathrm{t}_{1 / 2}(\mathrm{calc})=0.86 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).
Hydrolysis: no hydrolyzable groups (Howard et al. 1991).
Oxidation: rate constants $\mathrm{k}<60 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}<6 \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982); photooxidation $t_{1 / 2}=0.321-3.21 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Biodegradation: aerobic $\mathrm{t}_{1 / 2}=14160-15600 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; quoted, Howard et al. 1991); anaerobic $t_{1 / 2}=56640-62400 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; quoted, Howard et al. 1991).
Biotransformation: estimated to be $3 \times 10^{-12} \mathrm{~mL}$ cell ${ }^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination ( $\mathrm{k}_{2}$ ) Rate Constants:
$\mathrm{k}_{1}=0.076-0.21 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0012-0.0014 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:
Air: $\mathrm{t}_{1 / 2}=0.321-3.21 \mathrm{~h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991); $\mathrm{t}_{1 / 2}=0.6 \mathrm{~h}$ for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated first order rate constant $\mathrm{k}=0.0179 \mathrm{~min}^{-1}$ at $1 \mathrm{cal} \mathrm{cm}^{-2} \mathrm{~min}^{-1}, 10 \mathrm{~g} / \mathrm{m}^{3} \mathrm{H}_{2} \mathrm{O}$ and $20^{\circ} \mathrm{C}$ (Kamens et al. 1988).
Surface water: $\mathrm{t}_{1 / 2}=14160-15600 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; quoted, Howard et al. 1991).
Groundwater: $\mathrm{t}_{1 / 2}=28320-31200 \mathrm{~h}$, based on aerobic soil die-away test data at $10-30^{\circ} \mathrm{C}$ (Coover \& Sims 1987; quoted, Howard et al. 1991).
Sediment:
Soil: $t_{1 / 2}=14160-15600 \mathrm{~h}$, based on aerobic soil die-away test data (Coover \& Sims 1987; quoted, Howard et al. 1991);
$\mathrm{t}_{1 / 2}>50 \mathrm{~d}$ (Ryan et al. 1988);
mean $t_{1 / 2}=9.1 \mathrm{yr}$ for Luddington soil (Wild et al. 1991).
Biota: elimination $\mathrm{t}_{1 / 2}=12.4 \mathrm{~d}$ from Oyster, $\mathrm{t}_{1 / 2}=4.8 \mathrm{~d}$ from clam Mercenario mercenaria (quoted, Meador et al. 1995).

TABLE 4.1.1.49.1
Reported Henry's law constants of benzo[ghi]perylene at various temperatures
ten Hulscher et al. 1992
gas stripping-HPLC/fluo.

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{H} /\left(\mathbf{P a ~ m} \mathbf{~ m}^{3} / \mathbf{m o l}\right)$ |
| :--- | :---: |
| 10.0 | 0.019 |
| 20.0 | 0.027 |
| 35.0 | 0.052 |
| 40.1 | 0.054 |
| 45.0 | 0.066 |
| 55.0 | 0.087 |
| enthalpy of volatilization: |  |
| $\Delta \mathrm{H}_{\text {vol }} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=26.1 \pm 1.0$ |  |
| entropy of volatilization, $\Delta \mathrm{S}$ |  |
| $\mathrm{T} \Delta \mathrm{S}_{\text {vol }} /\left(\mathrm{kJ} \cdot \mathrm{mol}^{-1}\right)=15.9 \pm 1.3$ |  |
|  |  |
| $\ln \mathrm{~K}_{\mathrm{AW}}=-\Delta \mathrm{H}_{\mathrm{vol}} / \mathrm{RT}+\Delta \mathrm{S}_{\text {vol }} / \mathrm{R}$ |  |
| $\mathrm{R}=8.314 \mathrm{~Pa} \mathrm{~m}^{3} \mathrm{~mol}^{-1} \mathrm{~K}^{-1}$ |  |

### 4.1.1.50 Indeno[1,2,3-cd] pyr .



Common Name: Indeno[1,2,3-cd]pyrene
Synonym: 2,3-o-phenylenepyrene,
Chemical Name: indeno[1,2,3-cd]pyrene
CAS Registry No: 193-39-5
Molecular Formula: $\mathrm{C}_{22} \mathrm{H}_{12}$
Molecular Weight: 276.330
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
162 (Lide 2003)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
233.8 (Ruelle \& Kesselring 1997, Passivirta et al. 1999) 283.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 21.51 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ : 49.41, 36.0 (exptl., calculated-group additivity method, Chickos et al. 1999) 56.5 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0453\left(\mathrm{mp}\right.$ at $162^{\circ} \mathrm{C}$ ) 0.043 (Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations):
0.00019 (generator column-HPLC/UV, Wise et al. 1981)
0.000438 ; $0.0023,0.000191$ (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997) $\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-0.758-1631 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations):
$1.33 \times 10^{-7}$ (estimated, Callahan et al. 1979)
$1.00 \times 10^{-8} ; 2.32 \times 10^{-7}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.56-6126 /(\mathrm{T} / \mathrm{K})($ solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.60-4839 /(\mathrm{T} / \mathrm{K})($ supercooled liquid, Passivirta et al. 1999)
Henry's Law Constant $\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right.$ at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$0.029^{*} \quad\left(20^{\circ} \mathrm{C}\right.$, gas stripping-HPLC/fluorescence, measured range $10-55^{\circ} \mathrm{C}$, ten Hulscher et al. 1992) $\log [\mathrm{H} /(\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol})]=10.36-3208 /(\mathrm{T} / \mathrm{K})($ Passivirta et al. 1999)
$0.0285 \quad\left(20^{\circ} \mathrm{C}\right.$, selected from reported experimentally measured values, Staudinger \& Roberts 1996, 2001) $\log \mathrm{K}_{\mathrm{AW}}=0.033-1455 /(\mathrm{T} / \mathrm{K})($ van't Hoff eq. derived from literature data, Staudinger \& Roberts 2001)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
7.66 (calculated $\pi$ substituent const., Callahan et al. 1979)
8.20 (calculated, Broman et al. 1991)
6.72 (calculated, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
8.00 (Baltic Sea particulate field samples, conen distribution-GC/MS, Broman et al. 1991)
$6.93\left(10^{\circ} \mathrm{C}\right), 6.88,6.84\left(20^{\circ} \mathrm{C}\right), 6.42\left(35^{\circ} \mathrm{C}\right), 6.32,6.31\left(45^{\circ} \mathrm{C}\right)\left(\log \mathrm{K}_{\mathrm{DOC}}-\right.$ dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers \& ten Hulscher 1996)
$6.80 \quad\left(20^{\circ} \mathrm{C}, \log \mathrm{K}_{\text {POC }}-\right.$ particulate organic material from lake, Lüers \& ten Hulscher 1996)

Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Bioconcentration and Uptake and Elimination Rate Constants ( $\mathrm{k}_{1}$ and $\mathrm{k}_{2}$ ):
$\mathrm{k}_{1}=0.067-0.20 \mathrm{mg} \mathrm{g}^{-1} \mathrm{~h}^{-1} ; \mathrm{k}_{2}=0.0010-0.0013 \mathrm{~h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:


### 4.1.1.51 Dibenz[a,c]anthracene



Common Name: Dibenz[a,c]anthracene
Synonym: 1,2:3,4-Dibenzanthracene, naphtho-2' , 3':9,10-phenanthrene
Chemical Name: dibenz[ $a, c]$ anthracene
CAS Registry No: 215-58-7
Molecular Formula: $\mathrm{C}_{22} \mathrm{H}_{14}$
Molecular Weight: 278.346
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
205 (Bjørseth 1983; Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
518 (Weast 1982-83)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ): 299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ : 25.82 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
46.65, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0171\left(\mathrm{mp}\right.$ at $205^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.0016 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$1.30 \times 10^{-9 *}$ (effusion method, extrapolated, De Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=16.25-7322.2 /(\mathrm{T} / \mathrm{K})$; temp range: $152-179^{\circ} \mathrm{C}$ (torsion-effusion, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=16.011-7207.2 /(\mathrm{T} / \mathrm{K})$; temp range: $152-179^{\circ} \mathrm{C}$ (weighing-effusion, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=16.131-7265 /(\mathrm{T} / \mathrm{K})$; temp range: $152-179^{\circ} \mathrm{C}$ (mean, de Kruif 1980)
$3.44 \times 10^{-7}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-5094 /(\mathrm{T} / \mathrm{K})+10.62 ; \Delta \mathrm{H}_{\text {vap }}=-97.5 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
7.19 (calculated, Miller et al. 1985)
7.11 (calculated-MCI $\chi$ as per Rekker \& De Kort 1979, Ruepert et al. 1985)
7.19 (recommended, Sangster 1989, 1993)
7.11 (TLC retention time correlation, De Voogt et al. 1990)
8.0068 (calculated-UNIFAC group contribution, Chen et al. 1993)
6.17 (recommended, Hansch et al. 1995)
$6.40 \pm 0.19,6.48 \pm 0.78$ (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{Oc}}$ :
6.54 (humic acid, HPLC-k' correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Air: half-lives under simulated atmospheric conditions: $\mathrm{t}_{1 / 2}-9.20 \mathrm{~h}$ in simulated sunlight, $\mathrm{t}_{1 / 2}=4.60 \mathrm{~h}$ in simulated sunlight + ozone ( 0.2 ppm ), $\mathrm{t}_{1 / 2}=3.82 \mathrm{~h}$ in dark reaction ozone ( 0.2 ppm ) (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983).

TABLE 4.1.1.51.1
Reported vapor pressures of dibenz[a,c]anthracene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
(1a)
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
de Kruif 1980
torsion-, weighing effusion

| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| :--- | :---: |
| 151.65 | 0.1 |
| 158.52 | 0.2 |
| 163.08 | 0.3 |
| 166.38 | 0.4 |
| 168.97 | 0.5 |
| 171.11 | 0.6 |
| 172.94 | 0.7 |
| 174.53 | 0.8 |
| 175.95 | 0.9 |
| 177.22 | 1.0 |
| 298.15 | $1.3 \times 10^{-9}$ |
|  | extrapolated |

$\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=138.0$


FIGURE 4.1.1.51.1 Logarithm of vapor pressure versus reciprocal temperature for dibenz[a,c]anthracene.

### 4.1.1.52 Dibenz[a,h]anthracene



Common Name: Dibenz $[a, h]$ anthracene
Synonym: DB[a,h]A, 1,2,5,6-dibenzanthracene, 1,2:5,6-dibenzanthracene
Chemical Name: 1,2:5,6-dibenzanthracene
CAS Registry No: 53-70-3
Molecular Formula: $\mathrm{C}_{22} \mathrm{H}_{14}$
Molecular Weight: 278.346
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
269.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
524 (Weast 1977)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
252.6 (Ruelle \& Kesselring 1997; Passivirta et al. 1999)
299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
31.165 (Ruelle \& Kesselring 1997)
31.16 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
58.26, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)
57.3 (Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.00399 (mp at $269.5^{\circ} \mathrm{C}$ ) 0.00389 (calculated, Passivirta et al. 1999)

Water Solubility ( $\mathrm{g} / \mathrm{m}^{3}$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated and the reported temperature dependence equations):
$0.0005 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942)
0.0006 (shake flask-UV, Klevens 1950)
0.0025 (shake flask-LSC, Means et al. 1980b)
0.00056 (lit. mean, Pearlman et al. 1984)
$\log \left[\mathrm{S}_{\mathrm{L}} /(\mathrm{mol} / \mathrm{L})\right]=-1.409-1631 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$1.33 \times 10^{-8}\left(20^{\circ} \mathrm{C}\right.$, estimated, Callahan et al. 1979)
$3.70 \times 10^{-10 *}$ (effusion method, De Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=16.049-7395.4 /(\mathrm{T} / \mathrm{K})$; temp range: $163-189^{\circ} \mathrm{C}$ (torsion-effusion, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=15.876-7312 /(\mathrm{T} / \mathrm{K})$; temp range: $163-189^{\circ} \mathrm{C}$ (weighing-effusion, de Kruif 1980)
$\log (\mathrm{P} / \mathrm{Pa})=15.962-7730 /(\mathrm{T} / \mathrm{K})$; temp range: $163-189^{\circ} \mathrm{C}$ (mean, de Kruif 1980)
$4.25 \times 10^{-10}$ (extrapolated-Antoine eq., Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.515-7420 /(\mathrm{T} / \mathrm{K})$; temp range 403-513 K (Antoine eq., Stephenson \& Malanowski 1987) $3.70 \times 10^{-10} ; 9.31 \times 10^{-8}$ (quoted solid $\mathrm{P}_{\mathrm{S}}$ from Mackay et al. 1992; converted to supercooled liquid $\mathrm{P}_{\mathrm{L}}$ with fugacity ratio F, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{Pa}\right)=12.82-5824 /(\mathrm{T} / \mathrm{K})$ (solid, Passivirta et al. 1999)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=9.82-5002 /(\mathrm{T} / \mathrm{K})$ (supercooled liquid, Passivirta et al. 1999)
$2.51 \times 10^{-7}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-5193 /(\mathrm{T} / \mathrm{K})+10.82 ; \Delta \mathrm{H}_{\text {vap }}=-99.4 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}{ }^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ and reported temperature dependence equations):
0.0074 (calculated-P/C, Mabey et al. 1982)
0.0076 (calculated-P/C, Eastcott et al. 1988)
$\log \left[\mathrm{H} /\left(\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}\right)\right]=11.23-3371 /(\mathrm{T} / \mathrm{K})$, (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{Ow}}$ :

```
6.50 (shake flask-LSC, Means et al. 1980b)
6.88 (HPLC-RT/MS, Burkhard et al. 1985)
5.80 (Hansch & Leo 1985)
6.75 \pm0.40 (recommended, Sangster 1989, 1993)
7.11 (TLC retention time correlation, De Voogt et al. 1990)
6.60 (shake flask-UV, pH 7.4, Alcorn et al. 1993)
6.50 (recommended, Hansch et al. 1995)
6.54\pm0.19, 6.60\pm0.78 (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
```

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:

```
5.84 (microorganisms-water, calculated from K Kow, Mabey et al. 1982)
4 . 6 3 ~ ( a c t i v a t e d ~ s l u d g e , ~ F r e i t a g ~ e t ~ a l . ~ 1 9 8 4 )
3.38, 4.63,1.0 (algae, activated sludge, fish, Freitag et al. 1985)
4.00 (Daphnia magna, Newsted & Giesy 1987)
```

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
6.31 (average of 14 soil/sediment samples, equilibrium sorption isotherms by shake flask-LSC, Means et al. 1980b)
6.22, 6.18 (calculated-regression of $\mathrm{k}_{\mathrm{p}}$ versus substrate properties, calculated- $\mathrm{K}_{\mathrm{OW}}$, Means et al. 1980b)
6.22 ; 6.11, 5.30, 5.62 (quoted; calculated-K $\mathrm{K}_{\mathrm{ow}}$, calculated-S and mp, calculated-S, Karickhoff 1981)
6.52 (calculated- $\mathrm{K}_{\mathrm{OW}}$, Mabey et al. 1982)
5.20 (calculated, Pavlou 1987)
6.31; 6.44; 3.75-5.77 (soil, quoted exptl.; calculated-MCI ${ }^{1} \chi$, calculated-K ${ }_{\text {ow }}$ range, Sabljic 1987a,b)
5.77 (soil, calculated-K $\mathrm{K}_{\text {ow }}$ based on model of Karickhoff et al. 1979, Sabljic 1987b)
5.66 (soil, calculated- $\mathrm{K}_{\text {Ow }}$ based on model of Means et al. 1982, Sabljic 1987b)
4.60 (soil, calculated-K $\mathrm{K}_{\text {OW }}$ based on model of Chiou et al. 1983, Sabljic 1987b)
4.61 (soil, calculated-K Ow based on model of Kenaga 1980, Sabljic 1987b)
3.75 (soil, calculated-K $\mathrm{K}_{\mathrm{ow}}$ based on model of Briggs 1981, Sabljic 1987b)
6.22 (calculated-MCI ${ }^{1} \chi$, Sabljic et al. 1995)
6.44 (humic acid, HPLC-k' correlation, Nielsen et al. 1997)
6.00; 6.30 (soil, calculated-universal solvation model; quoted exptl., Winget et al. 2000)
6.76-8.42; 5.80-8.50 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss \& Wilcke 2001)
$6.03 ; 7.0,6.76,7.32\left(20^{\circ} \mathrm{C}\right.$, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3solvophobic approach, Krauss \& Wilcke 2001)

Environmental Fate Rate Constants, $k$ or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Volatilization:
Photolysis: atmospheric and aqueous photolysis $\mathrm{t}_{1 / 2}=782 \mathrm{~h}$, based on measured rate of photolysis in heptane
under November sunlight (Muel \& Saguim 1985; quoted, Howard et al. 1991) and $\mathrm{t}_{1 / 2}=6 \mathrm{~h}$ after adjusting the ratio of sunlight photolysis in water versus heptane (Smith et al. 1978; Muel \& Saguem 1985; quoted, Howard et al. 1991);
pseudo-first-order direct photolysis rate constant $\mathrm{k}($ exptl $)=0.014 \mathrm{~min}^{-1}$ with the calculated $\mathrm{t}_{1 / 2}=0.83 \mathrm{~h}$ and the predicted $\mathrm{k}=0.0216 \mathrm{~min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);
direct photolysis $\mathrm{t}_{1 / 2}(\mathrm{obs})=.0.31 \mathrm{~h}, \mathrm{t}_{1 / 2}=0.38 \mathrm{~h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Oxidation: rate constant $\mathrm{k}=5 \times 10^{8} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for singlet oxygen and $\mathrm{k}=1.5 \times 10^{4} \mathrm{M}^{-1} \mathrm{~h}^{-1}$ for peroxy radical (Mabey et al. 1982);
photooxidation $t_{1 / 2}=0.428-4.28 \mathrm{~h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis: not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).
Biodegradation: aerobic $\mathrm{t}_{1 / 2}=8664-22560 \mathrm{~h}$, based on aerobic soil die-away test data (Coover \& Sims 1987; Sims 1990; quoted, Howard et al. 1991);
$\mathrm{k}=0.0019 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=361 \mathrm{~d}$ for Kidman sandy loam and $\mathrm{k}=0.0017 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=420 \mathrm{~d}$ for McLarin sandy loam all at -0.33 bar soil moisture (Park et al. 1990).
Biotransformation: estimated to be $3 \times 10^{-12} \mathrm{~mL} \mathrm{cell}^{-1} \mathrm{~h}^{-1}$ for bacteria (Mabey et al. 1982).
Bioconcentration, Uptake ( $\mathrm{k}_{1}$ ) and Elimination $\left(\mathrm{k}_{2}\right)$ Rate Constants:

Half-Lives in the Environment:
Air: half-lives under simulated atmospheric conditions: $\mathrm{t}_{1 / 2}=9.6 \mathrm{~h}$ in simulated sunlight, $\mathrm{t}_{1 / 2}=4.8 \mathrm{~h}$ in simulated sunlight + ozone $(0.2 \mathrm{ppm}), \mathrm{t}_{1 / 2}=2.71 \mathrm{~h}$ in dark reaction ozone $(0.2 \mathrm{ppm})$ (Katz et al. 1979; quoted, Bjørseth \& Olufsen 1983);
$t_{1 / 2}=0.428-4.28 \mathrm{~h}$, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $\mathrm{t}_{1 / 2}=6-782 \mathrm{~h}$, based on sunlight photolysis half-life in water (Smith et al. 1978; Muel \& Saguem 1985; quoted, Howard et al. 1991);
photolysis $t_{1 / 2}=0.83 \mathrm{~h}$ in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996).
Groundwater: $t_{1 / 2}=17328-45120 \mathrm{~h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: biodegradation rate constant $\mathrm{k}=0.0019 \mathrm{~d}^{-1}$ with $\mathrm{t}_{1 / 2}=361 \mathrm{~d}$ for Kidman sandy loam soil and $\mathrm{k}=0.117 \mathrm{~d}^{-1}$ with $t_{1 / 2}=420 \mathrm{~d}$ for McLaurin sandy loam soil (Park et al. 1990);
$t_{1 / 2} \sim 8664-22560 \mathrm{~h}$, based on aerobic soil dieaway test data (Coover \& Sims 1987; Sims 1990; quoted, Howard et al. 1991); mean $t_{1 / 2}=20.607 \mathrm{wk}$ (quoted, Wild et al. 1991).
Biota:

## TABLE 4.1.1.52.1

Reported vapor pressures of dibenz[a,h]anthracene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
(1) $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
(2) $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$
de Kruif 1980

| torsion-, weighing effusion |  |
| :--- | :---: |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 160.38 | 0.1 |
| 168.21 | 0.2 |
| 172.93 | 0.3 |
| 176.33 | 0.4 |
| 179.01 | 0.5 |
| 181.22 | 0.6 |
| 183.11 | 0.7 |
| 184.76 | 0.8 |

TABLE 4.1.1.52.1 (Continued)
de Kruif 1980

| de Kruif $\mathbf{1 9 8 0}$ |  |
| :--- | :---: |
| torsion-, weighing effusion |  |
| $\mathbf{t} /{ }^{\circ} \mathbf{C}$ | $\mathbf{P} / \mathbf{P a}$ |
| 186.22 | 0.9 |
| 187.54 | 1.0 |
| 25.0 | $3.7 \times 10^{-10}$ |
|  | extrapolated |

$\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=140.0$


FIGURE 4.1.1.52.1 Logarithm of vapor pressure versus reciprocal temperature for dibenz[a,h]anthracene.

### 4.1.1.53 Dibenz[a,j]anthracene



Common Name: Dibenz[ $a, j$ ]anthracene
Synonym: 1,2:7,8-dibenzanthracene, 1,2:7,8-dibenzanthracene, a, $a^{\prime}$-dibenzanthracene, dinaphthanthracene Chemical Name: dibenz[a,j]anthracene
CAS Registry No: 58-70-3
Molecular Formula: $\mathrm{C}_{22} \mathrm{H}_{14}$
Molecular Weight: 278.346
Melting Point ( ${ }^{\circ} \mathrm{C}$ ): 197.5 (Lide 2003)

Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.20^{\circ} \mathrm{C}\right)$ :
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
222.8 (Ruelle \& Kesselring 1997)
299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.0203\left(\mathrm{mp}\right.$ at $197.5^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$0.012 \quad\left(27^{\circ} \mathrm{C}\right.$, shake flask-nephelometry, Davis et al. 1942; quoted, Shaw 1989)
0.012 (quoted, Yalkowsky et al. 1983; Pearlman et al. 1984)
$0.000041,0.00022$ (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)
Vapor Pressure $\left(\mathrm{Pa}\right.$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m} 3 / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{ow}}$ :
7.19 (calculated-fragment const., Yalkowsky et al. 1983)
7.11 (calculated-MCI $\chi$ as per Rekker \& De Kort 1979, Ruepert et al. 1985)
7.11 (TLC retention time correlation, De Voogt et al. 1990)
7.11 (quoted and recommended, Sangster 1993)
$6.54 \pm 0.19,6.44 \pm 0.75$ (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997; quoted, Nielsen et al. 1997)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log$ BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
6.58 (humic acid, HPLC-k' correlation, Nielsen et al. 1997)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 4.1.1.54 Pentacene



Common Name: Pentacene
Synonym: 2,3,6,7-dibenzanthracene, 2,3:6,7-dibenzanthracene
Chemical Name: pentacene
CAS Registry No: 135-48-8
Molecular Formula: $\mathrm{C}_{22} \mathrm{H}_{14}$
Molecular Weight: 278.346
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
270-271 (Weast 1982-83)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
290-300 (sublimation, Weast 1982-83)
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
299.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
35.19 (Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
55.22, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: $0.00395\left(\mathrm{mp}\right.$ at $270^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
$1.0 \times 10^{-13 *}$ (effusion method, De Kruif 1980)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=12.725-8260 /(\mathrm{T} / \mathrm{K})$; temp range $444-566 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
$1.19 \times 10^{-12 *}$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $170-210^{\circ} \mathrm{C}, \mathrm{Oja}$ \&
Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=35.823-18867 /(\mathrm{T} / \mathrm{K})$; temp range $443-483 \mathrm{~K}$ (Antoine eq., Knudsen effusion, Oja \& Suuberg 1998)
Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
7.19 (calculated -f const., Miller et al. 1985)
7.19 (recommended, Sangster 1989, 1993)
7.11 (TLC retention time correlation, De Voogt et al. 1990)
8.0068 (calculated-UNIFAC group contribution, Chen et al. 1993)
7.19 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 4.1.1.54.1
Reported vapor pressures of pentacene at various temperatures and the coefficients for the vapor pressure equations
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$
$\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$

| de Kruif 1980 |  | Oja \& Suuberg 1998 |  |
| :---: | :---: | :---: | :---: |
| torsion-, weighing effusion |  | Knudsen effusion |  |
| t/ ${ }^{\circ} \mathrm{C}$ | P/Pa | t/ ${ }^{\circ} \mathrm{C}$ | $\mathbf{P / P a}$ |
| 220.51 | 0.1 | 171.33 | 0.00161 |
| 229.8 | 0.2 | 184.8 | 0.00413 |
| 235.4 | 0.3 | 185.99 | 0.00421 |
| 239.45 | 0.4 | 190.98 | 0.00760 |
| 242.63 | 0.5 | 200.29 | 0.0171 |
| 245.27 | 0.6 | 203.1 | 0.0157 |
| 247.51 | 0.7 | 212.6 | 0.0515 |
| 249.47 | 0.8 |  |  |
| 251.22 | 0.9 | $\mathrm{mp} / \mathrm{K}$ | > 573 |
| 252.79 | 1.0 |  |  |
| 25.0 | $1.0 \times 10^{-13}$ | eq. 1a | $\mathrm{P} / \mathrm{Pa}$ |
|  | extrapolated | A | 35.823 |
|  |  | B | 18823 |
| $\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=155.0$ |  | for temp $\Delta \mathrm{H}_{\text {subl }} /(\mathrm{k}$ | $\begin{aligned} & 443-483 \mathrm{~K} \\ & -1.155 .9 \end{aligned}$ |



FIGURE 4.1.1.54.1 Logarithm of vapor pressure versus reciprocal temperature for pentacene.

### 4.1.1.55 Coronene



Common Name: Coronene
Synonym: hexabenzobenzene
Chemical Name: coronene
CAS Registry No: 191-07-1
Molecular Formula: $\mathrm{C}_{24} \mathrm{H}_{12}$
Molecular Weight: 300.352
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
$437.4 \quad$ (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
525 (Weast 1982-83; Stephenson \& Malanowski 1987; Lide 2003)
Density $\left(\mathrm{g} / \mathrm{cm}^{3}\right.$ at $\left.25^{\circ} \mathrm{C}\right)$ : 1.371 (Lide 2003)

Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
244.8 (Ruelle \& Kesselring 1997)
$219.1 \quad\left(25^{\circ} \mathrm{C}\right.$, calculated-density)
292.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
19.202 (Ruelle \& Kesselring 1997)
19.2 (exptl., Chickos et al. 1999)

Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
27.02, 42.8 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 8.99 \times 10^{-5}\left(\mathrm{mp}\right.$ at $\left.437.4^{\circ} \mathrm{C}\right)$
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
0.00014 (shake flask-fluorescence, Mackay \& Shiu 1977)
0.00014 (average lit. value, Pearlman et al. 1984)
0.00010 (generator column-HPLC/UV, Billington et al. 1988)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
$\log (\mathrm{P} / \mathrm{mmHg})=12.62-7675 /(\mathrm{T} / \mathrm{K})$; temp range $160-240^{\circ} \mathrm{C}$ (Knudsen effusion method, Hoyer \& Peperle 1958) $1.95 \times 10^{-10}$ (Knudsen effusion method, extrapolated, Murray et al. 1974)
$\log (\mathrm{P} / \mathrm{atm})=9.110-7100 /(\mathrm{T} / \mathrm{K})$; temp range $427-510 \mathrm{~K}$ (Knudsen effusion method, Murray et al. 1974)
$2.00 \times 10^{-10}$ (extrapolated-Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=11.1157-7100 /(\mathrm{T} / \mathrm{K})$; temp range $427-510 \mathrm{~K}$ (solid, Antoine eq.-I, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{S}} / \mathrm{kPa}\right)=8.886-5764 /(\mathrm{T} / \mathrm{K})$; temp range not specified (solid, Antoine eq.-II, Stephenson \& Malanowski 1987)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=8.318-5362 /(\mathrm{T} / \mathrm{K})$; temp range not specified (liquid, Antoine eq.-III, Stephenson \& Malanowski 1987)
$2.89 \times 10^{-10 *}$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range $148-231^{\circ} \mathrm{C}, \mathrm{Oja} \&$ Suuberg 1998)
$\log (\mathrm{P} / \mathrm{Pa})=31.72-16006 /(\mathrm{T} / \mathrm{K})$; temp range 421-504 K (Antoine eq., Knudsen effusion, Oja \& Suuberg 1998)
$2.55 \times 10^{-8}$ (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, calibrated GC-RT correlation, Lei et al. 2002)
$\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-5446 /(\mathrm{T} / \mathrm{K})+10.67 ; \Delta \mathrm{H}_{\text {vap }}=-104.2 \mathrm{~kJ} \cdot \mathrm{~mol}^{-1}(\mathrm{GC}-\mathrm{RT}$ correlation, Lei et al. 2002)

Henry's Law Constant ( $\mathrm{Pa} \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
7.64 (average lit. value, Yalkowsky et al. 1983)
7.64 (calculated-MCI $\chi$ as per Rekker \& De Kort 1979, Ruepert et al. 1985)
8.20, 6.70 (HPLC-RV correlation, different mobile phases, Brooke et al. 1986)
5.40 (shake flask/slow stirring-GC, Brooke et al. 1986)
6.50 (recommended, Sangster 1989, 1993)
7.64 (TLC retention time correlation, De Voogt et al. 1990)
8.0 (calculated-K $\mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)
5.40, 6.70 (Hansch et al. 1995)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
7.80 (Baltic Sea particulate field samples, conen distribution-GC/MS, Broman et al. 1991)
5.0 (predicted dissolved $\log \mathrm{K}_{\mathrm{OC}}$, Broman et al. 1991)

Environmental Fate Rate Constants, k or Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:
Soil: mean $t_{1 / 2}=16.5$ yr for Luddington soil (Wild et al. 1991).

TABLE 4.1.1.55.1
Reported vapor pressures of coronene at various temperatures and the coefficients for the vapor pressure equations

| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ | $(1)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})$ |
| ---: | :--- | ---: | :--- |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ | $(2)$ |  | $\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)$ |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})$ | $(3)$ |  |  |
| $\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})$ | (4) |  |  |


| Hoyer \& Peperle 1958 | Murray et al. 1974 | Oja \& Suuberg 1998 |
| :---: | :---: | :---: |
| effusion | Knudsen effusion | Knudsen effusion |
| $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathrm{P} / \mathbf{P a}$ | $\mathbf{t} /{ }^{\circ} \mathrm{C} \quad \mathbf{P} / \mathbf{P a}$ |
| data presented by equation | data presented by graph and | 147.9 0.00191 |
| eq. $1 \quad \mathrm{P} / \mathrm{mmHg}$ | eq. $1 \quad \mathrm{P} / \mathrm{atm}$ | 163.60 .00686 |
| A 12.62 | A 9.110 | 178.10 .0236 |
| B 7676 | B 7100 | 196.90 .0895 |
| for temp range $160-240^{\circ} \mathrm{C}$ | for temp range 427-510 K | 109.9 0.222 |
|  |  | 210.0 0.309 |
| $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ} / \mathrm{mol})=147.0$ | $\begin{array}{ll} 25.0 & 2.0 \times 10^{-10} \\ \text { extrapolated } \end{array}$ | 231.110 .927 |
|  | $\mathrm{mp} /{ }^{\circ} \mathrm{C}$ | $\mathrm{mp} / \mathrm{K}$ |
|  |  | eq. 1a $\mathrm{P} / \mathrm{Pa}$ |
|  | $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ} / \mathrm{mol})=135.9$ | A 31.72 |
|  | at av. temp measurements | B 16006 |
|  |  | temp range 421-504 K |
|  |  | $\Delta \mathrm{H}_{\text {sub }} /(\mathrm{kJ} / \mathrm{mol})=133.1$ |



FIGURE 4.1.1.55.1 Logarithm of vapor pressure versus reciprocal temperature for coronene.

### 4.1.2 Chlorinated polynuclear aromatic hydrocarbons

### 4.1.2.1 2,4",5-Trichloro-p-terphenyl



Common Name: 2,4",5-Trichloro-p-terphenyl
Synonym:
Chemical Name:
CAS Registry No: 61576-93-0
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{11} \mathrm{Cl}_{3}$
Molecular Weight: 333.639
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
92 (Dickhut et al. 1994)
Boiling Point $\left({ }^{\circ} \mathrm{C}\right)$ :
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
335.9 (calculated-Le Bas method at normal boiling point)

Heat of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.22 ( mp at $92^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$3.8 \times 10^{-4} ; 3.37 \times 10^{-4}$ (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)
$1.01 \times 10^{-4}, 6.56 \times 10^{-4}, 8.56 \times 10^{-4}\left(5,25,30^{\circ} \mathrm{C}\right.$, generator column-GC, Dickhut et al. 1994)
Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ ):
Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{oc}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 4.1.2.2 2,4,4",6-Tetrachloro-p-terphenyl



Common Name: 2,4,4",6-Tetrachloro-p-terphenyl
Synonym:
Chemical Name:
CAS Registry No:
Molecular Formula: $\mathrm{C}_{18} \mathrm{H}_{11} \mathrm{Cl}_{4}$
Molecular Weight: 368.084
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
114 (Dickhut et al. 1994)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
Density ( $\mathrm{g} / \mathrm{cm}^{3}$ ):
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
356.8 (calculated-Le Bas method at normal boiling point)

Heat of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$ (assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$ ), F: 0.134 (m.p at $114^{\circ} \mathrm{C}$ )
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $25^{\circ} \mathrm{C}$ or as indicated):
$1.79 \times 10^{-4} ; 7.91 \times 10^{-5}$ (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)
$5.91 \times 10^{-5}, 1.74 \times 10^{-4}, 4.07 \times 10^{-4}\left(5,25,40^{\circ} \mathrm{C}\right.$, generator column-GC, Dickhut et al. 1994)
Vapor Pressure (Pa at $25^{\circ} \mathrm{C}$ ):
Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ ):
Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\text {ow }}$ :
Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ :
Bioconcentration Factor, $\log \mathrm{BCF}$ or $\log \mathrm{K}_{\mathrm{B}}$ :
Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

### 4.1.3 Polychlorinated naphthalenes

### 4.1.3.1 1-Chloronaphthalene



Common Name: 1-Chloronaphthalene
Synonym: PCN-1, $\alpha$-chloronaphthalene
Chemical Name: 1-chloronaphthalene
CAS Registry No: 90-13-1
Molecular Formula: $\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Cl}$
Molecular Weight: 162.616
Melting Point ( ${ }^{\circ} \mathrm{C}$ ):
-2.5 (Lide 2003)
Boiling Point ( ${ }^{\circ} \mathrm{C}$ ):
259 (Lide 200)
Density (g/cm ${ }^{3}$ ):
$1.1938 \quad\left(20^{\circ} \mathrm{C}\right.$, Weast 1982-83; Windholz 1983; Budavari 1989)
1.1976, $1.1938\left(15^{\circ} \mathrm{C}, 20^{\circ} \mathrm{C}\right.$, Riddick et al. 1986)
$1.188 \quad\left(25^{\circ} \mathrm{C}\right.$, Lide 2003)
Molar Volume ( $\mathrm{cm}^{3} / \mathrm{mol}$ ):
$136.2 \quad\left(20^{\circ} \mathrm{C}\right.$, calculated-density)
168.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, $\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})$ :
Entropy of Fusion, $\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})$ :
Fugacity Ratio at $25^{\circ} \mathrm{C}$, F: 1.0
Water Solubility $\left(\mathrm{g} / \mathrm{m}^{3}\right.$ or $\mathrm{mg} / \mathrm{L}$ at $\left.25^{\circ} \mathrm{C}\right)$ :
22.4 (shake flask-fluorescence, Mackay \& Shiu 1981)
19.0; 8.93 (quoted; calculated-molecular connectivity indices, Nirmalakhandan \& Speece 1989)
2.87 (quoted, Crookes \& Howe 1993, Alcock et al. 1999)
6.75; 36.3 (quoted exptl value; calculated-molar volume, Wang et al. 1992)
19.1; 25.8 (quoted; calculated-group contribution method, Kühne et al. 1995)
19.1; 25.2 (quoted; calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated $*$ are compiled at the end of this section):
133.3* $\quad\left(80.6^{\circ} \mathrm{C}\right.$, static-Hg manometer, measured range $80.6-269.3^{\circ} \mathrm{C}$, Kahlbaum 1898)
133.3* $\quad\left(80.6^{\circ} \mathrm{C}\right.$, summary of literature data, temp range $80.6-269.3^{\circ} \mathrm{C}$, Stull 1947)
3.055 (extrapolated from Antoine eq., temp range 353-533 K, Stephenson \& Malanowski 1987)
$\log (\mathrm{P} / \mathrm{kPa})=6.15143-[1861.65 /(\mathrm{T} / \mathrm{K}-83.337)]$; temp range: $353-533 \mathrm{~K}$ (Antoine eq., Stephenson \& Malanowski 1987)
2.133 (estimated, Crookes \& Howe 1993)
$1.2 \times 10^{-4}$ (estimated, Alcock et al. 1999)
3.597, 3.84 (calibrated GC-RT correlation, GC-RT correlation, $\mathrm{P}_{\mathrm{L}}$ supercooled liquid values, Lei et al. 1999) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3058 /(\mathrm{T} / \mathrm{K})+10.81$ (HPLC-RT correlation, Lei et al. 1999)
5.588 (supercooled liquid $\mathrm{P}_{\mathrm{L}}$, regression with GC-RT from literature, Lei et al. 1999) $\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3054 /(\mathrm{T} / \mathrm{K})+9.97$; (regression with GC-RT from literature, supercooled liquid, Lei et al. 1999) $6.89^{*} \quad\left(23.15^{\circ} \mathrm{C}\right.$, transpiration method, measured range 289.1-332.3 K, Verevkin 2003)
$\ln \left(\mathrm{P} / \mathrm{P}^{\mathrm{o}}\right)=299.001 / \mathrm{R}-83941.481 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(73.5 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]$, where $\mathrm{P}^{\mathrm{o}}=101.325 \mathrm{kPa}$, gas constant $\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}$ (vapor pressure eq. from transpiration measurement, temp range $289.1-332.3 \mathrm{~K}$, Verevkin 2003)

Henry's Law Constant ( $\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}$ at $25^{\circ} \mathrm{C}$ ):
35.5 (gas stripping-GC, Mackay \& Shiu 1981)
36.3 (gas stripping-GC, Shiu \& Mackay 1997)

Octanol/Water Partition Coefficient, $\log \mathrm{K}_{\mathrm{OW}}$ at $25^{\circ} \mathrm{C}$ and the reported temperature dependence equations:
3.80 (HPLC-k'correlation, Hanai et al. 1981)
4.08 (calculated-fragment constant, Yalkowsky et al. 1983)
3.90 (shake flask, Opperhuizen 1987)
4.08 (estimated, Abernethy \& Mackay 1987)
3.80 (calculated-molar volume, Wang et al. 1992)
4.24 (recommended, Hansch et al. 1995)
4.0; 3.97 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
$\log \mathrm{K}_{\mathrm{OW}}=0.841+940.09 /(\mathrm{T} / \mathrm{K})$, temp range $5-55^{\circ} \mathrm{C}$ (temperature dependence HPLC-k'correlation, Lei et al. 2000)
4.06 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log \mathrm{K}_{\mathrm{OA}}$ at $25^{\circ} \mathrm{C}$ or as indicated and reported temperature dependence equations:
$6.39,6.10,5.52,5.30,5.13\left(10,20,30,40,50^{\circ} \mathrm{C}\right.$, GC-RT correlation, Su et al. 2002) $\log \mathrm{K}_{\mathrm{OA}}=58300 /(2.303 \cdot \mathrm{RT})-4.40$; temp range $10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}$ correlation, Su et al. 2002)

Bioconcentration Factor, $\log$ BCF or $\log \mathrm{K}_{\mathrm{B}}$ :
2.28 (Cyprinus carpio, for monochloronaphthalenes, Matsuo 1984; quoted, Crookes \& Howe 1993)

Sorption Partition Coefficient, $\log \mathrm{K}_{\mathrm{OC}}$ :
2.97 (estimated for mono-chloronaphthalenes, Crookes \& Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, $\mathrm{t}_{1 / 2}$ :
Half-Lives in the Environment:

TABLE 4.1.3.1.1
Reported vapor pressures of 1 -chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations

```
log P = A - B/(T/K)
log P = A - B/(C + t/ }\mp@subsup{}{}{\circ}\textrm{C}
log P = A - B/(C + T/K)
log P = A - B/(T/K) - C}\cdot\operatorname{log}(T/K
(4a)


TABLE 4.1.3.1.1 (Continued)
\begin{tabular}{|c|c|c|c|c|c|}
\hline \multicolumn{2}{|r|}{Kahlbaum 1898} & \multicolumn{2}{|c|}{Stull 1947} & \multicolumn{2}{|l|}{Verevkin 2003} \\
\hline \multicolumn{2}{|r|}{static-Hg manometer} & \multicolumn{2}{|l|}{summary of lit. data} & \multicolumn{2}{|l|}{transpiration-GC} \\
\hline t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa \\
\hline 159.3 & 6666 & 230.8 & 53329 & 32.15 & 14.07 \\
\hline 171.4 & 9999 & 269.3 & 101325 & 35.35 & 18.30 \\
\hline 180.4 & 13332 & & & 38.35 & 24.71 \\
\hline 204.2 & 26664 & \(\mathrm{mp} /{ }^{\circ} \mathrm{C}\) & -20 & 40.35 & 28.10 \\
\hline 218.3 & 39997 & & & 41.15 & 29.56 \\
\hline 230.8 & 53329 & & & 44.05 & 35.53 \\
\hline 240.5 & 66661 & & & 47.05 & 46.62 \\
\hline 248.6 & 79993 & & & 50.15 & 55.93 \\
\hline 255.5 & 93326 & & & 53.15 & 69.72 \\
\hline \multirow[t]{9}{*}{269.3} & 101325 & & & 56.15 & 84.66 \\
\hline & & & & 59.15 & 105.54 \\
\hline & & & & eq. 4 a & \(\mathrm{P} / \mathrm{kPa}\) \\
\hline & & & & \(\mathrm{P}^{0}\) & 101.325 kPa \\
\hline & & & & A & 299.011/R \\
\hline & & & & B & 83941.481/R \\
\hline & & & & C & 73.5/R \\
\hline & & & & \(\mathrm{R}=8.3\) & \(\mathrm{K}^{-1} \mathrm{~mol}^{-1}\) \\
\hline & & & & \[
\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}
\] & \[
\begin{aligned}
& -1)=62.03 \\
& \text { at } 298.15 \mathrm{~K}
\end{aligned}
\] \\
\hline
\end{tabular}


FIGURE 4.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1 -chloronaphthalene.

\subsection*{4.1.3.2 2-Chloronaphthalene}


Common Name: 2-Chloronaphthalene
Synonym: PCN-2, \(\beta\)-chloronaphthalene
Chemical Name: 2-chloronaphthalene
CAS Registry No: 91-58-7
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Cl}\)
Molecular Weight: 162.616
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
58 (Lide 2003)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
256 (Weast 1982-83; Windholz 1983; Budavari 1989; Järnberg et al. 1994; Lide 2003)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
\(1.1377 \quad\left(71^{\circ} \mathrm{C}\right.\), Weast 1982-83; Lide 2003)
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
\(142.9 \quad\left(71^{\circ} \mathrm{C}\right.\), calculated from density, Stephenson \& Malanowski 1987)
168.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
3.346 (Ruelle \& Kesselring 1997)

Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.474\left(\mathrm{mp}\right.\) at \(58^{\circ} \mathrm{C}\) )
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) ):
11.7 (shake flask-fluorescence, Mackay \& Shiu 1981)
0.924 (shake flask, Opperhuizen et al. 1985, 1986)
8.93 (calculated-molecular connectivity indices, Nirmalakhandan \& Speece 1989)
16.3 (calculated-group contribution method, Kühne et al. 1995)
7.80 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \(*\) are compiled at the end of this section):
5.34 (supercooled liquid value, extrapolated from Antoine eq., temperature range \(400-435 \mathrm{~K}\), Stephenson \& Malanowski 1987)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=7.8608-[3021.2 /(\mathrm{T} / \mathrm{K})]\); temp range \(400-435 \mathrm{~K}\) (Antoine eq., Stephenson \& Malanowski 1987) \(3.679,3.84\) (supercooled liquid values \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation, GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3054 /(\mathrm{T} / \mathrm{K})+10.81(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
2.526 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3054 /(\mathrm{T} / \mathrm{K})+9.97\) (regression with GC-RT data from literature, Lei et al. 1999)
2.301* \(\quad\left(24.15^{\circ} \mathrm{C}\right.\), transpiration method, measured range \(280.2-330.7 \mathrm{~K}\), Verevkin 2003)
\(\ln \left(\mathrm{P} / \mathrm{P}^{\circ}\right)=301.255 / \mathrm{R}-87496.950 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(39.5 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\), where \(\mathrm{P}^{\mathrm{o}}=101.325 \mathrm{kPa}\), gas constant \(\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}\) (vapor pressure eq. from transpiration measurement, solid, temp range 280.2-330.7 K, Verevkin 2003)
53.71* \(\quad\left(59.05^{\circ} \mathrm{C}\right.\), transpiration method, measured range \(332.2-362.2 \mathrm{~K}\), Verevkin 2003)
\(\ln \left(\mathrm{P} / \mathrm{P}^{0}\right)=294.501 / \mathrm{R}-84197.803 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(73.5 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\), where \(\mathrm{P}^{\mathrm{o}}=101.325 \mathrm{kPa}\), gas constant
\(\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}\) (vapor pressure eq. from transpiration measurements, liquid, temp range 332.2-362.2
K, Verevkin 2003)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
31.9 (gas stripping-GC, Mackay \& Shiu 1981)
33.5 (gas stripping-GC, Shiu \& Mackay 1997)

Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
4.80 (calculated-fragment constant, Yalkowsky et al. 1983)
4.19 (HPLC-RT correlation, Opperhuizen et al. 1985, 1986)
4.08 (estimated, Abernethy \& Mackay 1987)
3.98 (shake flask, Opperhuizen 1987)
4.07 (selected, Isnard \& Lambert 1988; 1989)
4.6024 (calculated-UNIFAC group contribution, Chen et al. 1993)
4.14 (selected, Hansch et al. 1995)
3.90; 3.91 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\text {ow }}=0.821+924.42 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC-k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations.
Additional data at other temperatures designated * are compiled at the end of this section:
\(6.36,6.08,5.50,5.28,5.11\left(10,20,30,40,50^{\circ} \mathrm{C}, \mathrm{GC}-\mathrm{RT}\right.\) correlation, Su et al. 2002)
\(\log \mathrm{K}_{\mathrm{OA}}=58000 /(2.303 \cdot \mathrm{RT})-4.40\); temp range \(10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}\) correlation, Su et al. 2002)
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
2.28 (Cyprinus carpio, for monochloronaphthalenes, Matsuo 1981)
3.63 (guppies, Opperhuizen et al. 1985)
3.63, 4.81 (whole fish, fish lipid, Gobas et al. 1987)
4.52 (guppy, lipid-weight based, Gobas et al. 1989)
3.63; 3.06 (quoted means; calculated- \(\mathrm{K}_{\text {ow }}\) and \(\mathrm{S}_{0}\), Banerjee \& Baughman 1991)
3.63 (Poecilia reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996)
2.496, 2.721 (calculated-MCI \(\chi\), calculated- \(\mathrm{K}_{\mathrm{ow}}\), Lu et al. 1999)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
2.97 (estimated for monochloronaphthalenes, Crookes \& Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Volatilization:
Photolysis:
Photooxidation:
Hydrolysis: laboratory determined hydrolysis rate constant \(\mathrm{k}=(9.5 \pm 2.8) \times 10^{-6} \mathrm{~h}^{-1}\) at neutral conditions, calculated \(\mathrm{t}_{1 / 2}=8.3 \mathrm{yr}\) at pH 7 (Ellington et al. 1988).
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=7.3 \times 10^{2} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=3.1 \times 10^{-1} \mathrm{~d}^{-1}\) (guppy, Opperhuizen et al. 1985; quoted, Connell \& Hawker 1988) \(\log \mathrm{k}_{1}=2.83 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-0.51 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)

Half-Lives in the Environment:
Air:
Surface water:
Ground water:
Sediment:
Soil: experimentally measured abiotic disappearance \(\mathrm{t}_{1 / 2}=11.3 \mathrm{~d}\) in two different soil types, a Captina silt loam (Typic Fragiudult) and McLaurin sandy loam (Typic Paleudults) (Anderson et al. 1991).
Biota: \(\mathrm{t}_{1 / 2}=2.3 \mathrm{~d}\) (female guppies, Opperhuizen et al. 1985, quoted, Crookes \& Howe 1993)

TABLE 4.1.3.2.1
Reported vapor pressures of 2-chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})\)
\(\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})\)
(1a)
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\)
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})\)
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})\)
\(\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\)
\(\ln \mathrm{P} / \mathrm{P}^{\mathrm{O}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\)
\begin{tabular}{|c|c|c|c|}
\hline \multicolumn{4}{|c|}{Verevkin 2003} \\
\hline \multicolumn{4}{|c|}{transpiration-GC} \\
\hline t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa \\
\hline & solid & & liquid \\
\hline 7.05 & 0.342 & 59.05 & 53.71 \\
\hline 10.15 & 0.494 & 62.05 & 64.43 \\
\hline 15.05 & 0.881 & 65.05 & 77.53 \\
\hline 17.05 & 1.103 & 68.05 & 95.98 \\
\hline 19.05 & 1.394 & 71.05 & 111.91 \\
\hline 21.05 & 1.716 & 74.05 & 134.91 \\
\hline 24.15 & 2.301 & 77.05 & 161.0 \\
\hline 27.15 & 3.162 & 80.05 & 190.2 \\
\hline 29.05 & 3.854 & 83.05 & 223.41 \\
\hline 30.15 & 4.361 & 85.05 & 252.43 \\
\hline 32.05 & 5.167 & 89.05 & 310.78 \\
\hline 34.05 & 6.297 & & \\
\hline 36.05 & 7.569 & \(\Delta \mathrm{H}_{\mathrm{V}} /(\mathrm{kJ}\) & \(=62.3 \pm 1.1\) \\
\hline 38.05 & 9.386 & & at 298.15 K \\
\hline 40.05 & 10.941 & & \\
\hline 42.05 & 13.466 & eq. 4 a & \(\mathrm{P} / \mathrm{kPa}\) \\
\hline 44.04 & 15.786 & \(\mathrm{P}^{0}\) & 101.325 kPa \\
\hline 46.05 & 18,715 & A & 294.501/R \\
\hline 48.05 & 22.307 & B & 84197.803/R \\
\hline 50.05 & 26.990 & C & 73.5/R \\
\hline 52.05 & 31.158 & \(\mathrm{R}=8\) & \(\mathrm{K}^{-1} \mathrm{~mol}^{-1}\) \\
\hline 54.05 & 36.801 & & \\
\hline 56.05 & 43.420 & & \\
\hline 57.55 & 49.194 & & \\
\hline eq. 4 a & \(\mathrm{P} / \mathrm{kPa}\) & & \\
\hline \(\mathrm{P}^{\text {o }}\) & 101.325 kPa & & \\
\hline A & 301.255/R & & \\
\hline B & 87496.95/R & & \\
\hline C & 39.5/R & & \\
\hline \multicolumn{4}{|l|}{\[
\begin{array}{r}
\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{~mol}^{-1}\right)=75.72 \\
\text { at } 298.15 \mathrm{~K}
\end{array}
\]} \\
\hline
\end{tabular}

\subsection*{4.1.3.3 1,2-Dichloronaphthalene}


Common Name: 1,2-Dichloronaphthalene
Synonym: PCN-3
Chemical Name: 1,2-dichloronaphthalene
CAS Registry No: 2050-69-3
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\)
Molecular Weight: 197.061
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
36 (Lide 2003)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
295.6 (Lide 2003)

Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ): 1.3147 ( \(49^{\circ} \mathrm{C}\), Weast 1982-83; Lide 2003)
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
156 (Ruelle \& Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), \(\mathrm{F}: 0.78\left(\mathrm{mp}\right.\) at \(\left.36^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.137 (generator column-GC/ECD, Opperhuizen 1987)
4.31 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equations):
0.344; 0.333 (supercooled liquid \(P_{L}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3172(/ \mathrm{T} / \mathrm{K})+10.18 ;(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.301 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3172 /(\mathrm{T} / \mathrm{K})+10.11\) (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
4.40 (HPLC-RT correlation, Opperhuizen et al. 1985)
4.42 (shake flask, Opperhuizen 1987; quoted, Sangster 1993, Crookes \& Howe 1993, Hansch et al. 1995)
4.66 (selected, Alcock et al. 1999)
4.60; 4.45 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\mathrm{OW}}=1.064+1060.21 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC-k' correlation, Lei et al. 2000) 4.69 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations: 6.93 (generator column-GC, Harner \& Bidleman 1998) \(7.35,7.01,6.44,6.13,5.91\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), GC-RT correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=66000 /(2.303 \cdot \mathrm{RT})-4.800\); temp range \(10-50^{\circ} \mathrm{C}\) (GC-RT correlation, Su et al. 2002) 6.89; 7.01 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) : 3.40 (fish, Opperhuizen et al. 1985)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.4 1,4-Dichloronaphthalene}


Common Name: 1,4-Dichloronaphthalene Synonym: PCN-5
Chemical Name: 1,4-dichloronaphthalene
CAS Registry No: 1825-31-6
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\)
Molecular Weight: 197.061
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
67.5 (Lide 2003)

Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
288 (Lide 2003)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
156.0 (Ruelle \& Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: 0.383 ( mp at \(288^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.314 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.314 (generator column-GC/ECD, Opperhuizen et al. 1987)
4.02 (calculated-TSA, Dickhut et al. 1994)
1.98 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equations):
\[
0.173 \text { (estimated, Crookes \& Howe 1993) }
\]
\(9.98 \times 10^{-6}\) (estimated, Alcock et al. 1999)
0.428; 0.416(supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3067(/ \mathrm{T} / \mathrm{K})+9.92(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.353 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3067 /(\mathrm{T} / \mathrm{K})+10.17\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\text {ow }}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
4.88 (HPLC-RT correlation, Opperhuizen et al. 1985)
4.66 (shake flask, Opperhuizen 1987; quoted, Gobas et al. 1987; 1989; Clark et al. 1990; Sangster 1993;

Crookes \& Howe 1993; Hansch et al. 1995; Devillers et al. 1996; Alcock et al. 1999)
4.79 (calculated, Oliver \& Niimi 1984; Oliver 1987)
4.80; 4.57 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\text {ow }}=1.269+1049.8 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC-k' correlation, Lei et al. 2000)
4.56 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations:
6.93 (generator column-GC/MS, Harner \& Bidleman 1998)
\(7.52,7.13,6.72,6.38,6.13\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), generator column-GC/MS, Harner \& Bidleman 1998)
\(\log \mathrm{K}_{\mathrm{OA}}=-3.97+3248 /(\mathrm{T} / \mathrm{K})\), temp range: \(10-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998) 6.78; 6.91 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
3.75 (Oncorhynchus mykiss, Oliver \& Niimi 1984)
3.36 (female guppies, Opperhuizen et al. 1985)
3.80 (Opperhuizen et al. 1985)
4.04 (Opperhuizen et al. 1985)
3.36, 4.54 (guppies: whole fish, fish lipid, Gobas et al. 1987)
3.75 (rainbow trout, Oliver \& Niimi 1984; Oliver 1987)
5.18 (guppy, lipid-weight based, Gobas et al. 1989)
3.36; 4.63 (quoted means; calculated \(-\mathrm{K}_{\mathrm{OW}}\) and \(\mathrm{S}_{0}\), Banerjee \& Baughman 1991)
3.75 (Oncorhynchus mykiss, under flow-through condition, quoted Devillers et al. 1996)
3.36 (Poecilia reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Volatilization:
Photolysis:
Photooxidation: rate constant \(\mathrm{k}=5.8 \times 10^{-12} \mathrm{~cm}^{3}\) molecule \({ }^{-1} \mathrm{~s}^{-1}\) for the gas-phase reactions with OH radical at \(298 \pm 2 \mathrm{~K}\) (Atkinson 1989).
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants \(\left(\mathrm{k}_{1}\right.\) and \(\left.\mathrm{k}_{2}\right)\) :
\(\mathrm{k}_{1}=1.2 \times 10^{3} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=1.1 \times 10^{-1} \mathrm{~d}^{-1}\) (guppies, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=3.04 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-0.96 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: \(\mathrm{t}_{1 / 2}=6.2 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)

\subsection*{4.1.3.5 1,8-Dichloronaphthalene}


Common Name: 1,8-Dichloronaphthalene
Synonym: PCN-9
Chemical Name: 1,8-dichloronaphthalene
CAS Registry No: 2050-74-0
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\)
Molecular Weight: 197.061
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
89 (Weast 1982-83; Lide 2003)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
sublimation (Lide 2003)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
156.0 (Ruelle \& Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.236\left(\mathrm{mp}\right.\) at \(89^{\circ} \mathrm{C}\) )
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) ):
0.315 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.059 (generator column-GC/ECD, Opperhuizen et al. 1987)
0.309 (Isnard \& Lambert 1988, 1989; quoted, Crookes \& Howe 1993)
1.27 (calculated-molar volume mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equation):
0.198 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3169 /(\mathrm{T} / \mathrm{K})+9.93\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OW}}\) :
4.41 (HPLC-RT, Opperhuizen et al. 1985)
4.19 (shake flask-GC, Opperhuizen 1987; quoted, Sangster 1993; Hansch et al. 1995)
5.4348 (calculated-UNIFAC, Chen et al. 1993)
4.85 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
3.79 (guppies, Opperhuizen et al. 1985)
3.79. 4.96 (guppies: whole fish, fish lipid, Gobas et al. 1987)
4.95 (guppy, lipid-weight based, Gobas et al. 1989)
3.79 (Poecilia reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=9.8 \times 10^{2} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=1.6 \times 10^{-1} \mathrm{~d}^{-1}\) (guppies, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=2.97 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-0.80 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: elimination \(\mathrm{t}_{1 / 2}=4.3 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985; Crookes \& Howe 1993)

\subsection*{4.1.3.6 2,3-Dichloronaphthalene}


Common Name: 2,3-Dichloronaphthalene
Synonym: PCN-10
Chemical Name: 2,3-dichloronaphthalene
CAS Registry No: 2050-75-1
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\)
Molecular Weight: 197.061
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
120 (Weast 1982-83; Ruelle \& Kesselring 1997; Lide 2003)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
\(156.0 \quad\) (Ruelle \& Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.117\left(\mathrm{mp}\right.\) at \(120^{\circ} \mathrm{C}\) )
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) ):
0.0862 (generator column-GC/ECD, Opperhuizen et al. 1985; 1987)
0.623 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equation):
0.333 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3169 /(\mathrm{T} / \mathrm{K})+10.15\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) :
4.71 (HPLC-RT correlation, Opperhuizen et al. 1985)
4.51 (shake flask, Opperhuizen 1987)
4.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log\) BCF or \(\log K_{B}\) :
4.04 (guppies, Opperhuizen et al. 1985)
4.04, 5.22 (guppies: whole fish, fish lipid, Gobas et al. 1987)
5.08 (guppy, lipid-weight based, Gobas et al. 1989)
4.04 (Poecilia reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants \(\left(\mathrm{k}_{1}\right.\) and \(\left.\mathrm{k}_{2}\right)\) :
\(\mathrm{k}_{1}=1.6 \times 10^{3} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=1.4 \times 10^{-1} \mathrm{~d}^{-1}\) (guppies, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=3.05 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-0.85 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: elimination \(t_{1 / 2}=5.1 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)

\subsection*{4.1.3.7 2,7-Dichloronaphthalene}


Common Name: 2,7-Dichloronaphthalene
Synonym: PCN-12
Chemical Name: 2,7-dichloronaphthalene
CAS Registry No: 2198-77-8
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\)
Molecular Weight: 197.061
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
115 (Lide 2003)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
156.0 (Ruelle \& Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: 0.131 ( mp at \(115^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.236 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.235 (reported as 2,8-dichloronaphthalene, generator column-GC/ECD, Opperhuizen 1987)
0.699 (calculated-molar volume mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
0.344 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3169 /(\mathrm{T} / \mathrm{K})+10.16\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\text {ow }}\) :
4.81 (HPLC-RT correlation, Opperhuizen et al. 1985)
4.56 (shake flask-GC, Opperhuizen 1987)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation:
\(7.28,6.95,6.38,6.08,5.85\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), GC-RT correlation, Su et al. 2002)
\(\log \mathrm{K}_{\mathrm{OA}}=65400 /(2.303 \cdot \mathrm{RT})-4.80\); temp range \(10-50^{\circ} \mathrm{C}(\) GC-RT correlation, Su et al. 2002)
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
4.04 (guppies, Opperhuizen et al. 1985; Crookes \& Howe 1993, Lu et al. 1999)
4.04 (guppies: whole fish, fish lipid, Gobas et al. 1987)
5.11 (guppy, lipid-weight based, Gobas et al. 1989)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=1.6 \times 10^{3} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=1.4 \times 10^{-1} \mathrm{~d}^{-1}\) (guppies, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=3.08 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-0.85 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: depuration \(t_{1 / 2}=5.1 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)

\subsection*{4.1.3.8 1,2,3-Trichloronaphthalene}


Common Name: 1,2,3-Trichloronaphthalene
Synonym: PCN-13
Chemical Name: 1,2,3-trichloronaphthalene
CAS Registry No:50402-52-3
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{5} \mathrm{Cl}_{3}\)
Molecular Weight: 231.506
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
81-84 (Järnberg et al. 1994)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
210.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Sublimation, \(\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
\(0.071 ; 0.0652\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3551 /(\mathrm{T} / \mathrm{K})+10.76(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999) 0.0791 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3485 /(\mathrm{T} / \mathrm{K})+10.59\) (regression with GC-RT from literature, Lei et al. 1999)

Henry's Law Constant \(\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right.\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation: \(8.24,7.85,7.30,6.91,6.63\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), GC-RT correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=73200 /(2.303 \cdot \mathrm{RT})-5.20\); temp range \(10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}\) correlation, Su et al. 2002) 7.66; 7.72 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log\) BCF or \(\log K_{B}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.9 1,3,7-Trichloronaphthalene}


Common Name: 1,3,7-Trichloronaphthalene
Synonym: PCN-21
Chemical Name: 1,3,7-trichloronaphthalene
CAS Registry No: 55720-37-1
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{5} \mathrm{Cl}_{3}\)
Molecular Weight: 231.506
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
113 (Crookes \& Howe 1993)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ): 274
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
168.9 (Ruelle \& Kesselring 1997)
210.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), \(\mathrm{F}: 0.137\left(\mathrm{mp}\right.\) at \(113^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.0644 (generator column-GC/ECD, Opperhuizen et al. 1985, 1987)
0.049 (Opperhuizen et al. 1986)
2.85 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
0.127 (estimated, Crookes \& Howe 1993)
\(7.10 \times 10^{-6}\) (estimated, Alcock et al. 1999)
0.114 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3485 /(\mathrm{T} / \mathrm{K})+10.74\) (regression with GC-RT from literature, Lei et al. 1999)
\(0.0778-\mathrm{P}_{\mathrm{S}}, 0.359-\mathrm{P}_{\mathrm{L}}\) (estimated for trichloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
5.59 (HPLC-RT correlation, Opperhuizen et al. 1985)
5.60 (selected, Opperhuizen et al. 1986)
5.35 (shake flask, Opperhuizen 1987)
5.08 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
3.94 (Cyprinus carpio, for trichloronaphthalenes, Matsuo 1981)
4.43 (guppies, Opperhuizen et al. 1985)
4.43, 5.61 (guppies: whole fish, fish lipid, Gobas et al. 1987)
5.96 (guppy, lipid-weight based, Gobas et al. 1989)
4.08 (calculated- \(\mathrm{K}_{\text {Ow }}\) and solubility, Banerjee \& Baughman 1991)
4.43 (Poecilia reticulata, under static and semi-static conditions, Devillers et al. 1996)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=2.3 \times 10^{3} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=8.4 \times 10^{-2} \mathrm{~d}^{-1}\) (guppy, Opperhuizen et al. 1985)
\(\mathrm{k}_{1}=1.7 \times 10^{3} \mathrm{~d}^{-1}\) (estimated, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=3.14 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-1.64 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: \(\mathrm{t}_{1 / 2}=8.3 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)

\subsection*{4.1.3.10 1,2,3,4-Tetrachloronaphthalene}


Common Name: 1,2,3,4-Tetrachloronaphthalene
Synonym: PCN-27
Chemical Name: 1,2,3,4-tetrachloronaphthalene
CAS Registry No: 20020-02-4
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\)
Molecular Weight: 265.951
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
199 (Lide 2003)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
181.8 (Ruelle \& Kesselring 1997)
231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.0196\left(\mathrm{mp}\right.\) at \(\left.199^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00426 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.0042 (generator column-GC/ECD, Opperhuizen 1987)
0.0172 (calculated-AQUAFAC, Myrdal et al. 1995)
0.016 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equations):
0.0197; 0.0173 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3825 /(\mathrm{T} / \mathrm{K})+11.12 ;(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.0162 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3825 /(\mathrm{T} / \mathrm{K})+10.96\) (regression with GC-RT from literature, Lei et al. 1999)
\(0.00536-\mathrm{P}_{\mathrm{S}} ; 0.0975-\mathrm{P}_{\mathrm{L}}\) (estimated for tetrachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
5.94 (HPLC-RT correlation, Opperhuizen et al. 1985)
5.90 (HPLC-RT correlation, Opperhuizen et al. 1985)
5.75 (shake flask-GC, Opperhuizen 1987)
6.30; 5.76 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\mathrm{OW}}=1.832+1347.46 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC- \(\mathrm{k}^{\prime}\) correlation, Lei et al. 2000)
5.91 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equation:
\(9.03,8.59,8.05,7.59,7.26\left(10,20,30,40,50^{\circ} \mathrm{C}, \mathrm{GC}-\mathrm{RT}\right.\) correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=79500 /(2.303 \cdot \mathrm{RT})-5.60\); temp range \(10-50^{\circ} \mathrm{C}\) (GC-RT correlation, Su et al. 2002) 8.30; 8.29 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
3.94 (Cyprinus carpio, Matsuo 1981)
3.71 (Oncorhynchus mykiss, Oliver \& Niimi 1984)
4.52 (guppies, Opperhuizen et al. 1985)
4.50 (fish, Opperhuizen et al. 1985)
4.66, 5.71 (whole fish, fish lipid, Gobas et al. 1987)
3.71 (rainbow trout, mean value, Oliver \& Niimi 1985)
5.96 (guppy, lipid-weight based, Gobas et al. 1989)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=3.3 \times 10^{3} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=9.9 \times 10^{-2} \mathrm{~d}^{-1}\) (guppy, Opperhuizen et al. 1985)
\(\mathrm{k}_{1}=1.3 \times 10^{3} \mathrm{~d}^{-1}\) (estimated, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=3.70 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-1.08 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: \(t_{1 / 2}=7\) d (guppies, Opperhuizen et al. 1985; quoted, Crookes \& Howe 1993)

\subsection*{4.1.3.11 1,2,3,5-Tetrachloronaphthalene}


Common Name: 1,2,3,5-Tetrachloronaphthalene
Synonym: PCN-28
Chemical Name: 1,2,3,5-tetrachloronaphthalene
CAS Registry No: 53555-63-8
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\)
Molecular Weight: 265.951
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
141 (Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Sublimation, \(\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.0728\left(\mathrm{mp}\right.\) at \(141^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
0.0203; 0.0179 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3836 /(\mathrm{T} / \mathrm{K})+11.17\); (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.0205 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3800 /(\mathrm{T} / \mathrm{K})+11.06\) (regression with GC-RT data from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\text {ow }}\) :
5.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equation:
\(8.98,8.55,8.00,7.55,7.22\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), GC-RT correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=79100 /(2.303 \cdot \mathrm{RT})-5.60\); temp range \(10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}\) correlation, Su et al. 2002) 8.29; 8.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{oc}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.12 1,3,5,7-Tetrachloronaphthalene}


Common Name: 1,3,5,7-Tetrachloronaphthalene
Synonym: PCN-42
Chemical Name: 1,3,5,7-tetrachloronaphthalene
CAS Registry No: 53555-64-9
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\)
Molecular Weight: 265.951
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
\(179 \quad\) (Crookes \& Howe 1993)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
181.8 (Ruelle \& Kesselring 1997)
231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.0308\left(\mathrm{mp}\right.\) at \(179^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00426 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.0040 (generator column-GC/ECD, Opperhuizen 1987)
0.0237 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
\(0.0480 \quad\) (estimated, Crookes \& Howe 1993)
\(2.70 \times 10^{-6} \quad\) (estimated, Alcock et al. 1999)
0.0415 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3800 /(\mathrm{T} / \mathrm{K})+11.36\) (regression with GC-RT from literature, Lei et al. 1999)
\(0.00536-\mathrm{P}_{\mathrm{S}} ; 0.0975-\mathrm{P}_{\mathrm{L}}\) (estimated for tetrachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) :
6.38 (HPLC-RT correlation, Opperhuizen et al. 1985)
6.40 (Opperhuizen 1986)
6.19 (shake flask, Opperhuizen 1987; selected, Hansch et al. 1995)
5.54 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equation:
8.39 (estimated value for tetrachloronaphthalenes, Kaupp \& McLachlan 1999)
\(8.58,8.18,7.62,7.21,6.90\left(10,20,30,40,50^{\circ} \mathrm{C}, \mathrm{GC}-\mathrm{RT}\right.\) correlation, Su et al. 2002)
\(\log \mathrm{K}_{\mathrm{OA}}=75000 /(2.303 \cdot \mathrm{RT})-5.40\); temp range \(10-50^{\circ} \mathrm{C}\) (GC-RT correlation, Su et al. 2002)
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
4.53 (guppies, Opperhuizen et al. 1985)
4.50 (guppies, Opperhuizen et al. 1985)
5.06, 5.71 (guppies: whole fish, fish lipid, Gobas et al. 1987)
5.81 (guppy, lipid-weight based, Gobas et al. 1989)
4.53; 4.37 (quoted means; calculated- \(\mathrm{K}_{\mathrm{Ow}}\) and S , Banerjee \& Baughman 1991)
4.701, 4.961 (calculated-MCI \(\chi\), calculated- \(\mathrm{K}_{\mathrm{Ow}}\), Lu et al. 1999)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :

Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=7.5 \times 10^{2} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=2.2 \times 10^{-2} \mathrm{~d}^{-1}\) (guppies, Opperhuizen et al. 1985)
\(\log \mathrm{k}_{1}=2.97 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-1.66 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)

Half-Lives in the Environment:
Biota: \(\mathrm{t}_{1 / 2}=30 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985)

\subsection*{4.1.3.13 1,3,5,8-Tetrachloronaphthalene}


Common Name: 1,3,5,8-Tetrachloronaphthalene
Synonym: PCN-43
Chemical Name: 1,3,5,8-tetrachloronaphthalene
CAS Registry No: 31604-28-1
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\)
Molecular Weight: 265.951
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
131 (Crookes \& Howe 1993; Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
181.8 (Ruelle \& Kesselring 1997)
231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.0912\left(\mathrm{mp}\right.\) at \(\left.131^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00825 (generator column-GC/ECD, Opperhuizen et al. 1985)
0.0030 (Opperhuizen 1986)
0.0082 (generator column-GC/ECD, Opperhuizen 1987)
0.0716 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
0.0208 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-3800 /(\mathrm{T} / \mathrm{K})+11.07\) (regression with GC-RT from literature, Lei et al. 1999)
\(0.00536-\mathrm{P}_{\mathrm{S}} ; 0.0975-\mathrm{P}_{\mathrm{L}}\) (estimated for tetrachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, log \(\mathrm{K}_{\mathrm{ow}}\) :
5.96 (HPLC-RT correlation, Opperhuizen et al. 1985; selected, Sangster 1993)
6.00 (Opperhuizen et al. 1985; Opperhuizen 1986)
5.76 (shake flask, Opperhuizen 1987; selected, Hansch et al. 1995)
5.81 (selected, Gobas et al. 1987, 1989)
5.78 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations:
8.39 (value for tetrachloronaphthalenes, Kaupp \& McLachlan 1999)
\(8.98,8.55,8.00,7.55,7.22\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), GC-RT correlation, Su et al. 2002)
\(\log \mathrm{K}_{\mathrm{OA}}=79100 /(2.303 \cdot \mathrm{RT})-5.60\); temp range \(10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}\) correlation, Su et al. 2002)
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
4.40 (guppies, Opperhuizen et al. 1985)
4.69, 5.57 (guppies: whole fish, fish lipid, Gobas et al. 1987)
5.62 (guppy, lipid-weight based, Gobas et al. 1989)
4.701, 4.582 (calculated-MCI \(\chi\), calculated- \(\mathrm{K}_{\mathrm{OW}}\), Lu et al. 1999)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{oc}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\mathrm{k}_{1}=1.2 \times 10^{3} \mathrm{~d}^{-1} ; \mathrm{k}_{2}=4.5 \times 10^{-2} \mathrm{~d}^{-1} \quad\) (guppies, Opperhuizen et al. 1985)
\(\mathrm{k}_{1}=1.4 \times 10^{3} \mathrm{~d}^{-1} \quad\) (fish, Opperhuizen 1986)
\(\log \mathrm{k}_{1}=3.10 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-1.35 \mathrm{~d}^{-1} \quad\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: \(\mathrm{t}_{1 / 2}=15.5 \mathrm{~d}\) (guppies, Opperhuizen et al. 1985)

\subsection*{4.1.3.14 1,2,3,4,6-Pentachloronaphthalene}


Common Name: 1,2,3,4,6-Pentachloronaphthalene
Synonym: PCN-50
Chemical Name: 1,2,3,4,6-pentachloronaphthalene
CAS Registry No: 67922-25-2
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{3} \mathrm{Cl}_{5}\)
Molecular Weight: 300.396
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
147 (Crookes \& Howe 1993; Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Sublimation, \(\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: 0.0635 (mp at \(147^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure (Pa at \(25^{\circ} \mathrm{C}\) ):
0.00562 ; 0.00475 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4123 /(\mathrm{T} / \mathrm{K})+11.58 ;(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999) 0.0055 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4116 /(\mathrm{T} / \mathrm{K})+11.55\) (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
7.0; 6.27 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000) \(\log \mathrm{K}_{\mathrm{Ow}}=2.166+1446.69 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC-k' correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and the reported temperature dependence equations: 8.91 (generator column-GC/MS, Harner \& Bidleman 1998) \(9.73,9.20,8.63,8.11,7.75\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), generator column-GC/MS, Harner \& Bidleman 1998) \(\log \mathrm{K}_{\mathrm{OA}}=-6.63+4629 /(\mathrm{T} / \mathrm{K})\), temp range: \(10-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998) 8.92; 8.85 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.15 1,2,3,5,7-Pentachloronaphthalene}


Common Name: 1,2,3,5,7-Pentachloronaphthalene Synonym: PCN-52
Chemical Name: 1,2,3,5,7-pentachloronaphthalene
CAS Registry No: 53555-65-0
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{3} \mathrm{Cl}_{5}\)
Molecular Weight: 300.396
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
171 (Crookes \& Howe 1993; Järnberg et al. 1994)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
313 (estimated, Crookes \& Howe 1993)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.0369\left(\mathrm{mp}\right.\) at \(\left.171^{\circ} \mathrm{C}\right)\)
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) ):
0.0073 (estimated, Crookes \& Howe 1993)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
\(4.266 \times 10^{-3}\) (estimated, Crookes \& Howe 1993)
\(2.40 \times 10^{-6}\) (estimated, Alcock et al. 1999)
\(0.00696 ; 0.00593\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4082 /(\mathrm{T} / \mathrm{K})+11.53(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.00798 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4082 /(\mathrm{T} / \mathrm{K})+11.71\) (regression with GC-RT data from literature, Lei et al. 1999)
\(0.0-133-\mathrm{P}_{\mathrm{S}} ; 0.0277-\mathrm{P}_{\mathrm{L}}\) (estimated for pentachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
5.46 (selected, Hawker 1990)
6.87 (estimated, Crookes \& Howe 1993, quoted, Alcock et al. 1999)
6.87 (quoted, Falandysz et al. 1997)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations:
8.73 (generator-column-GC, Harner \& Bidleman 1998)
9.50, 9.04, 8.47, 7.97, 7.63 (10, 20, 30, \(40,50^{\circ} \mathrm{C}\), generator column-GC/MS, Harner \& Bidleman 1998) \(\log \mathrm{K}_{\mathrm{OA}}=-6.02+4394 /(\mathrm{T} / \mathrm{K})\); temp range: \(10-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998)
9.00 (estimated, Kaupp \& McLachlan 1999)
8.82; 8.76 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log\) BCF or \(\log \mathrm{K}_{\mathrm{B}}\) :
4.23 (selected, Hawker 1990)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
4.36 (estimated, Crookes \& Howe 1993)

Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.16 1,2,3,5,8-Pentachloronaphthalene}


Common Name: 1,2,3,5,8-Pentachloronaphthalene Synonym: PCN-53
Chemical Name: 1,2,3,5,8-pentachloronaphthalene
CAS Registry No: 150224-24-1
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{3} \mathrm{Cl}_{5}\)
Molecular Weight: 300.396
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
174-176 (Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
252.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Sublimation, \(\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations):
\(0.00394 ; 0.00329\) (supercooled liquid \(P_{L}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4204 /(\mathrm{T} / \mathrm{K})+11.70(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999) 0.00428 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4116 /(\mathrm{T} / \mathrm{K})+11.44\) (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) at \(25^{\circ} \mathrm{C}\) and the temperature dependence equations:
6.80; 6.13 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000) \(\log \mathrm{K}_{\mathrm{Ow}}=2.305+1431.02 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC-k' correlation, Lei et al. 2000)
6.46 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations:
9.13 (generator column-GC/MS, Harner \& Bidleman 1998)
9.97, 9.44, 8.86, 8.34, 7.96 (10, 20, 30, \(40,50^{\circ} \mathrm{C}\), generator column-GC/MS, Harner \& Bidleman 1998)
\(\log \mathrm{K}_{\mathrm{OA}}=-6.59+4684 /(\mathrm{T} / \mathrm{K})\); temp range: \(10-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998)
9.10; 9.01 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.17 1,2,3,4,5,7-Hexachloronaphthalene}


Common Name: 1,2,3,4,5,7-Hexachloronaphthalene
Synonym: PCN-64
Chemical Name: 1,2,3,4,5,7-hexachloronaphthalene
CAS Registry No: 67927-67-4
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\)
Molecular Weight: 334.842
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
194 (Crookes \& Howe 1993)
164-166 (Järnberg et al. 1994)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
331 (estimated, Crookes \& Howe 1993)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.022\left(\mathrm{mp}\right.\) at \(\left.194^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00011 (estimated, Crookes \& Howe 1993)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
\(9.47 \times 10^{-4} \quad\) (estimated, Crookes \& Howe 1993)
\(5.30 \times 10^{-8}\) (estimated, Alcock et al. 1999)
0.00134 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4432 /(\mathrm{T} / \mathrm{K})+11.99\) (regression with GC-RT data from literature, Lei et al. 1999)
\(0.000257-\mathrm{P}_{\mathrm{S}} ; 0.00809-\mathrm{P}_{\mathrm{L}}\) (estimated for hexachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):

Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
7.58 (estimated, Crookes \& Howe 1993, quoted, Alcock et al. 1999)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and the reported temperature dependence equations: 9.80 (generator-column-GC, Harner \& Bidleman 1998)
\(10.07,9.57,8.95,8.54\left(20,30,40,50^{\circ} \mathrm{C}\right.\), generator column-GC/MS, Harner \& Bidleman 1998) \(\log \mathrm{K}_{\mathrm{OA}}=-6.77+4393 /(\mathrm{T} / \mathrm{K})\); temp range: \(20-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998) 10.02 (value for hexachloronaphthalenes, Kaupp \& McLachlan 1999)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.18 1,2,3,4,6,7-Hexachloronaphthalene}


Common Name: 1,2,3,4,6,7-Hexachloronaphthalene Synonym: PCN-66
Chemical Name: 1,2,3,4,6,7-hexachloronaphthalene
CAS Registry No: 103426-96-6
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\)
Molecular Weight: 334.842
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
205-206 (Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Sublimation, \(\Delta \mathrm{H}_{\text {subl }}(\mathrm{kJ} / \mathrm{mol})\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations):
\(0.0015 ; 0.00121\) (supercooled liquid \(P_{L}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4411 /(\mathrm{T} / \mathrm{K})+11.97(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.00157 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4432 /(\mathrm{T} / \mathrm{K})+12.06\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) at \(25^{\circ} \mathrm{C}\) and the temperature dependence equations:
7.70; 6.79 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\mathrm{OW}}=2.489+1556.37 /(\mathrm{T} / \mathrm{K})\); temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC- \(\mathrm{k}^{\prime}\) correlation, Lei et al. 2000)
6.77 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations: 9.70 (generator column-GC/MS, Harner \& Bidleman 1998)
\(10.58,10.01,9.46,8.84,8.42\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), generator column-GC/MS, Harner \& Bidleman 1998)
\(\log \mathrm{K}_{\mathrm{OA}}=-7.09+5003 /(\mathrm{T} / \mathrm{K})\); temp range: \(10-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998)
9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.19 1,2,3,5,6,7-Hexachloronaphthalene}


Common Name: 1,2,3,5,6,7-Hexachloronaphthalene
Synonym: PCN-67
Chemical Name: 1,2,3,5,6,7-hexachloronaphthalene
CAS Registry No: 103426-97-7
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\)
Molecular Weight: 334.842
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
234-235 (Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure (Pa at \(25^{\circ} \mathrm{C}\) ):
\(0.00150 ; 0.00121\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4411 /(\mathrm{T} / \mathrm{K})+11.97(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999) 0.00157 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT data from literature, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4432 /(\mathrm{T} / \mathrm{K})+12.06\) (regression with GC-RT data from literature, Lei et al. 1999)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation:
9.70 (generator column-GC.MS, Harner \& Bidleman 1998)
\(10.58,10.01,9.46,8.84,8.42\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), generator column-GC/MS, Harner \& Bidleman 1998) \(\log \mathrm{K}_{\mathrm{OA}}=-7.09+5003 /(\mathrm{T} / \mathrm{K})\); temp range: \(10-50^{\circ} \mathrm{C}\) (generator column-GC/MS, Harner \& Bidleman 1998) 9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.20 1,2,3,5,7,8-Hexachloronaphthalene}


Common Name: 1,2,3,5,7,8-Hexachloronaphthalene
Synonym: PCN-69
Chemical Name: 1,2,3,5,7,8-hexachloronaphthalene
CAS Registry No: 103426-94-4
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\)
Molecular Weight: 334.842
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
148-149 (Järnberg et al. 1994)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
273.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations):
\(0.00124 ; 0.0010\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4441 /(\mathrm{T} / \mathrm{K})+11.99(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.00134 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4432 /(\mathrm{T} / \mathrm{K})+11.99\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) at \(25^{\circ} \mathrm{C}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
7.50; 6.69 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\mathrm{OW}}=2.413+1535.48 /(\mathrm{T} / \mathrm{K})\); temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC- \(\mathrm{k}^{\prime}\) correlation, Lei et al.
2000)
6.87 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equation:
9.83 (generator column-GC.MS, Harner \& Bidleman 1998)
\(10.09,9.62,8.99,8.57\left(20,30,40,50^{\circ} \mathrm{C}\right.\), generator column-GC/MS, Harner \& Bidleman 1998) \(\log \mathrm{K}_{\mathrm{OA}}=-6.64+4909 /(\mathrm{T} / \mathrm{K})\); temp range: \(20-50^{\circ} \mathrm{C}\) (generator column-GC, Harner \& Bidleman 1998) 9.67; 9.53 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.21 1,2,3,4,5,6,7-Heptachloronaphthalene}


Common Name: 1,2,3,4,5,6,7-Heptachloronaphthalene
Synonym: PCN-73
Chemical Name: 1,2,3,4,5,6,7-heptachloronaphthalene
CAS Registry No: 58863-14-2
Molecular Formula: \(\mathrm{C}_{10} \mathrm{HCl}_{7}\)
Molecular Weight: 369.287
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
293.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :

Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00062 (generator column-GC/ECD, Opperhuizen 1985; quoted, Opperhuizen 1986)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equations):
\(5.44 \times 10^{-4}-\mathrm{P}_{\mathrm{S}} ; 0.00258-\mathrm{P}_{\mathrm{L}}\) (estimated for heptachloronaphthalenes, Kaupp \& McLachlan 1999)
\(2.93 \times 10^{-4}, 2.78 \times 10^{-4}\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4745 /(\mathrm{T} / \mathrm{K})+12.38(\mathrm{GC}-\mathrm{RT}\) correlation, supercooled liquid, Lei et al. 1999)
0.000278 (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4745 /(\mathrm{T} / \mathrm{K})+12.37\) (regression with GC-RT from literature, Lei et al. 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations:
8.20 (HPLC-RT, Opperhuizen et al. 1985; quoted, Opperhuizen 1986)
7.69 (calculated-fragment const., Burreau et al. 1997)
8.20; 7.18 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000) \(\log \mathrm{K}_{\mathrm{ow}}=2.638+1660.82 /(\mathrm{T} / \mathrm{K})\); temp range \(5-55^{\circ} \mathrm{C}\left(\right.\) HPLC \(-\mathrm{k}^{\prime}\) correlation, Lei et al. 2000)
7.33 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equation:
\(11.52,10.96,10.44,9.75,9.28\left(10,20,30,40,50^{\circ} \mathrm{C}, \mathrm{GC}-\mathrm{RT}\right.\) correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=99500 /(2.303 \cdot \mathrm{RT})-6.80\); temp range \(10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}\) correlation, Su et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.22 1,2,3,4,5,6,8-Heptachloronaphthalene}


Common Name: 1,2,3,4,5,6,8-Heptachloronaphthalene
Synonym: PCN-74
Chemical Name: 1,2,3,4,5,6,8-heptachloronaphthalene
CAS Registry No: 58863-15-3
Molecular Formula: \(\mathrm{C}_{10} \mathrm{HCl}_{7}\)
Molecular Weight: 369.287
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
194 (Crookes \& Howe 1993; Järnberg et al. 1994)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
348 (estimated, Crookes \& Howe 1993)
Density \(\left(\mathrm{g} / \mathrm{cm}^{3}\right)\) :
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
293.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.022\left(\mathrm{mp}\right.\) at \(194^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00004 estimated, Crookes \& Howe 1993; quoted, Alcock et al. 1999)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equation):
\(3.73 \times 10^{-4} \quad\) (estimated, Crookes \& Howe 1993)
\(2.10 \times 10^{-8} \quad\) (estimated, Alcock et al. 1999)
\(2.46 \times 10^{-4} \quad\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-4748 /(\mathrm{T} / \mathrm{K})+12.31\) (regression with GC-RT from literature, Lei et al. 1999)
\(5.44 \times 10^{-4}-\mathrm{P}_{\mathrm{S}} ; 0.00258-\mathrm{P}_{\mathrm{L}}\) (estimated for heptachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
8.30 (estimated, Crookes \& Howe 1993, quoted, Alcock et al. 1999)
8.50; 7.46 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equation:
\(11.56,10.99,10.47,9.79,9.31\left(10,20,30,40,50^{\circ} \mathrm{C}, \mathrm{GC}-\mathrm{RT}\right.\) correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=99800 /(2.303 \cdot \mathrm{RT})-6.80\); temp range \(10-50^{\circ} \mathrm{C}\) (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.3.23 Octachloronaphthalene}


Common Name: Octachloronaphthalene
Synonym: PCN-75
Chemical Name: octachloronaphthalene
CAS Registry No: 2234-13-1
Molecular Formula: \(\mathrm{C}_{10} \mathrm{Cl}_{8}\)
Molecular Weight: 403.731
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
197.5 (Lide 2003)

Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
365 (estimated, Crookes \& Howe 1993)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
314.8 (calculated-Le Bas method at normal boiling point)
233.7 (Ruelle \& Kesselring 1997)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.0203\left(\mathrm{mp}\right.\) at \(197.5^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
\(0.000078,0.00008\) (generator column-GC/ECD, Opperhuizen 1986)
0.00008 (generator column-GC/ECD, Opperhuizen 1987)
0.00008; 0.00027 (quoted; calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equations):
\(1.33 \times 10^{-4}\) (estimated, Crookes \& Howe 1993)
\(7.50 \times 10^{-9}\) (estimated, Alcock et al. 1999)
\(7.61 \times 10^{-5}, 5.60 \times 10^{-5}\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\) : calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999) \(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-5021 /(\mathrm{T} / \mathrm{K})+12.72\) (Antoine eq., GC-RT correlation, supercooled liquid, Lei et al. 1999)
\(6.84 \times 10^{-5} \quad\) (supercooled liquid \(\mathrm{P}_{\mathrm{L}}\), regression with GC-RT from literature, Lei et al. 1999)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{Pa}\right)=-5021 /(\mathrm{T} / \mathrm{K})+12.82\) (regression with GC-RT from literature, Lei et al. 1999)
\(1.60 \times 10^{-5}-\mathrm{P}_{\mathrm{S}} ; 8.71 \times 10^{-4}-\mathrm{P}_{\mathrm{L}}\) (estimated for heptachloronaphthalenes, Kaupp \& McLachlan 1999)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) at \(25^{\circ} \mathrm{C}\) and the reported temperature dependence equations.
6.50 (calculated, Kaiser 1983)
8.40 (HPLC-RT correlation, Opperhuizen et al. 1985)
8.50 (Opperhuizen 1986)
6.42 (shake flask, Opperhuizen)
7.90 (calculated, Banerjee \& Baughman 1991)
8.50, 7.47 (calibrated HPLC- \(\mathrm{k}^{\prime}\) correlation, HPLC- \(\mathrm{k}^{\prime}\) correlation, Lei et al. 2000)
\(\log \mathrm{K}_{\mathrm{OW}}=2.998+1660.82 /(\mathrm{T} / \mathrm{K})\), temp range \(5-55^{\circ} \mathrm{C}\) (temperature dependence HPLC- \(\mathrm{k}^{\prime}\) correlation, Lei et al. 2000)
7.70 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) at \(25^{\circ} \mathrm{C}\) or as indicated and the reported temperature dependence equations: \(12.39,11.78,11.27,10.51,9.98\left(10,20,30,40,50^{\circ} \mathrm{C}\right.\), GC-RT correlation, Su et al. 2002) \(\log \mathrm{K}_{\mathrm{OA}}=10600 /(2.303 \cdot \mathrm{RT})-7.20\); temp range \(10-50^{\circ} \mathrm{C}(\mathrm{GC}-\mathrm{RT}\) correlation, Su et al. 2002)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
2.50 (Oncorhynchus mykiss, Oliver \& Niimi 1985; quoted, Crookes \& Howe 1993
2.52 (rainbow trout, mean value, Oliver \& Niimi 1985)
5.0 (calculated- \(\mathrm{K}_{\mathrm{ow}}\) and \(\mathrm{S}_{0}\), Banerjee \& Baughman 1991)
2.52 (Oncorhynchus mykiss, under flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{oc}}\) :
5.38 (estimated, Crookes \& Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Volatilization:
Photolysis:
Photooxidation: \(\mathrm{t}_{1 / 2}=1608-16082 \mathrm{~h}\) based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Hydrolysis:
Biodegradation: aerobic biodegradation \(\mathrm{t}_{1 / 2}=4320-8760 \mathrm{~h}\), based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin \& Chou 1981; quoted, Howard et al. 1991);
anaerobic biodegradation \(t_{1 / 2}=17280-35040 \mathrm{~h}\), based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin \& Chou 1981; quoted, Howard et al. 1991).
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
Half-Lives in the Environment:
Air: photooxidation \(t_{1 / 2}=1608-16082 \mathrm{~h}\) in air based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).
Surface water: \(\mathrm{t}_{1 / 2}=4320-8760 \mathrm{~h}\), based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin \& Chou 1981; quoted, Howard et al. 1991).
Ground water: \(\mathrm{t}_{1 / 2}=8640-17520 \mathrm{~h}\), based on essentially no biodegradation observed for hexachloro-benzene in soil die-away tests (Griffin \& Chou 1981; quoted, Howard et al. 1991).
Sediment:
Soil: \(\mathrm{t}_{1 / 2}=4320-8760 \mathrm{~h}\), based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin \& Chou 1981; quoted, Howard et al. 1991).
Biota:

\subsection*{4.1.4 Brominated polynuclear aromatic hydrocarbons}

\subsection*{4.1.4.1 1-Bromonaphthalene}


Common Name: 1-Bromonaphthalene
Synonym: \(\alpha\)-bromonaphthalene
Chemical Name: 1-bromonaphthalene
CAS Registry No: 90-11-9
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Br}\)
Molecular Weight: 207.067
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
6.1 (Lide 2003)

Boiling Point (C):
281 (Lide 2003)
Density \(\left(\mathrm{g} / \mathrm{cm}^{3}\right.\) at \(\left.20^{\circ} \mathrm{C}\right)\) :
1.4834 (Dean 1992)
1.4785 (Lide 2003)

Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
\(140.6\left(30^{\circ} \mathrm{C}\right.\), calculated from density, Stephenson \& Malanowski 1987)
\(140.0 \quad\left(20^{\circ} \mathrm{C}\right.\), calculated-density)
170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(\mathrm{pK}_{\mathrm{a}}\) :
Enthalpy of Vaporization, \(\Delta \mathrm{H}_{\mathrm{V}}(\mathrm{kJ} / \mathrm{mol})\) : 39.33 (at normal bp, Hon et al. 1976)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\), F: 1.0
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
9.95 (Yalkowsky et al. 1983)
7.72 (calculated-molecular connectivity indices, Nirmalakhandan \& Speece 1989)
\(9.08,9.80,13.35\), and \(18.98\left(4,10,25\right.\), and \(40^{\circ} \mathrm{C}\), generator column-UV spec., Dickhut et al. 1994)
25.3 (calculated-TSA, Dickhut et al. 1994)
14.0 (calculated-group contribution method, Kühne et al. 1995)
23.3 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
266.6* \(\quad\left(97.9^{\circ} \mathrm{C}\right.\), static- Hg manometer, measured range \(97.9-281.1^{\circ} \mathrm{C}\), Kahlbaum 1898)

133* (84.2 \({ }^{\circ} \mathrm{C}\), summary of literature data, temp range \(84.2-281.1^{\circ} \mathrm{C}\), Stull 1947)
\(\log (\mathrm{P} / \mathrm{mmHg})=[-0.2185 \times 13274.9 /(\mathrm{T} / \mathrm{K})]+8.131285\); temp range \(84.2-281.1^{\circ} \mathrm{C}\), (Antoine eq., Weast 1972-73)
18681* ( \(196.27^{\circ} \mathrm{C}\), ebulliometry, measured range \(97.9-285.92^{\circ} \mathrm{C}\), Hon et al. 1976)
\(\log (\mathrm{P} / \mathrm{mmHg})=5.38175-929.64 /\left(91.06+\mathrm{t} /{ }^{\circ} \mathrm{C}\right.\) ); temp range: \(196.27-285.93^{\circ} \mathrm{C}\) (Antoine eq., twin ebulliometry, Hon et al. 1976)
0.713*, 1.07* (torsion effusion, measured range 295-359 K, Urbani et al. 1980)
\(\log (\mathrm{P} / \mathrm{kPa})=(6.90-2950 /(\mathrm{T} / \mathrm{K})\), temp range 295-359 K (torsion and Knudsen effusion, Urbani et al. 1980)
\(\log (\mathrm{P} / \mathrm{mmHg})=7.00350-1927.05 /\left(186.0+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\); temp range: liquid (Antoine eq., Dean 1985, 1992)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=6.56365-2303.73 /[-48.841+(\mathrm{T} / \mathrm{K})]\); temp range \(357-555 \mathrm{~K}\) (liquid, Antoine eq.-I, Stephenson \& Malanowski 1987)
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=4.50679-929.871 /[182.045+(\mathrm{T} / \mathrm{K})]\), temp range \(469-559 \mathrm{~K}\), (liquid, Antoine eq.-II, Stephenson \& Malanowski 1987)
2.754* \(\quad\left(30.15^{\circ} \mathrm{C}\right.\), transpiration method, measured range \(303.3-336.3 \mathrm{~K}\), Verevkin 2003)
\(\ln \left(\mathrm{P} / \mathrm{P}^{\circ}\right)=299.001 / \mathrm{R}-8.3941 .481 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(73.5 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\), where \(\mathrm{P}^{\circ}=101.325 \mathrm{kPa}\), gas constant \(\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}\) (vapor pressure eq. from transpiration measurement, temp range \(303.3-336.3 \mathrm{~K}\), Verevkin 2003)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
4.35 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) or Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

TABLE 4.1.4.1.1
Reported vapor pressures of 1-bromonaphthalene at various temperatures and the coefficients for the vapor pressure equations
\[
\begin{align*}
& \log P=A-B /(T / K)  \tag{1}\\
& \log P=A-B /\left(C+t /{ }^{\circ} C\right)  \tag{2}\\
& \log P=A-B /(C+T / K)  \tag{3}\\
& \log P=A-B /(T / K)-C \cdot \log (T / K) \tag{4}
\end{align*}
\]
1.
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline \multicolumn{2}{|r|}{Kahlbaurm 1898} & \multicolumn{2}{|c|}{Stull 1947} & \multicolumn{2}{|l|}{Hon et al. 1976} & \multicolumn{2}{|l|}{Urbani et al. 1980} \\
\hline \multicolumn{2}{|l|}{static method-manometer} & \multicolumn{2}{|l|}{summary of literature data} & \multicolumn{2}{|r|}{ebulliometry} & \multicolumn{2}{|l|}{torsion effusion} \\
\hline t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa \\
\hline & & & & \multicolumn{4}{|c|}{Run A. 01} \\
\hline 97.9 & 266.6 & 84.2 & 133.3 & 196.27 & 18681 & 25 & 0.713 \\
\hline 117.5 & 666.6 & 117.5 & 666.6 & 213.14 & 28206 & 28 & 0.950 \\
\hline 134.0 & 1333 & 133.6 & 1333 & 228.08 & 39235 & 30 & 1.37 \\
\hline 151.3 & 2666 & 150.2 & 2666 & 234.45 & 44740 & 33 & 1.31 \\
\hline 157.2 & 3333 & 170.2 & 5333 & 244.51 & 54504 & 34 & 1.43 \\
\hline 162.3 & 3999 & 183.5 & 7999 & 245.13 & 55150 & 40 & 2.85 \\
\hline 166.7 & 4666 & 198.8 & 13332 & 250.71 & 61192 & 42 & 3.05 \\
\hline 170.5 & 5333 & 224.2 & 26664 & 256.24 & 67574 & 45 & 3.62 \\
\hline 177.1 & 6666 & 252.2 & 53329 & 262.78 & 75759 & 46 & 3.72 \\
\hline 189.6 & 9999 & 281.1 & 101325 & 275.35 & 93151 & 47 & 4.16 \\
\hline 198.8 & 13332 & & & 279.49 & 99510 & 48 & 4.51 \\
\hline 223.8 & 26664 & \(\mathrm{mp} /{ }^{\circ} \mathrm{C}\) & 5.5 & 281.40 & 102474 & 49 & 4.75 \\
\hline 239.7 & 39997 & & & 284.04 & 106737 & 50 & 4.99 \\
\hline 252.0 & 53329 & & & 285.92 & 109863 & 52 & 5.82 \\
\hline 261.6 & 66661 & & & & & 58 & 7.78 \\
\hline 269.8 & 79993 & & & \(\mathrm{bp} /{ }^{\circ} \mathrm{C}\) & 280.56 & 61 & 8.94 \\
\hline 277.2 & 93326 & & & & & 66 & 12.8 \\
\hline
\end{tabular}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline \multicolumn{8}{|l|}{TABLE 4.1.4.1.1 (Continued)} \\
\hline \multicolumn{2}{|r|}{Kahlbaurm 1898} & \multicolumn{2}{|c|}{Stull 1947} & \multicolumn{2}{|l|}{Hon et al. 1976} & \multicolumn{2}{|l|}{Urbani et al. 1980} \\
\hline \multicolumn{2}{|l|}{static method-manometer} & \multicolumn{2}{|l|}{summary of literature data} & \multicolumn{2}{|r|}{ebulliometry} & \multicolumn{2}{|l|}{torsion effusion} \\
\hline \(t /{ }^{\circ} \mathrm{C}\) & P/Pa & \(\mathrm{t}^{2} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & \(\mathrm{t}^{\circ} \mathrm{C}\) & P/Pa \\
\hline \multirow[t]{5}{*}{281.1} & 101325 & & & eq. 2 & P/mmHg & 74 & 20.2 \\
\hline & & & & A & 5.38157 & 77 & 24.3 \\
\hline & & & & B & 929.64 & 86 & 42.0 \\
\hline & & & & C & 91.06 & & \\
\hline & & & & \[
\Delta \mathrm{H}_{\mathrm{v}} / \mathrm{k} \text {. }
\] & \[
\begin{gathered}
-1)=39.33 \\
\text { at bp }
\end{gathered}
\] & & \\
\hline
\end{tabular}
2.

Urbani et al. 1980
(Continued) Verevkin 2003
\begin{tabular}{|c|c|c|c|c|c|}
\hline \multicolumn{2}{|c|}{(Continued)} & & & \multicolumn{2}{|r|}{Verevkin 2003} \\
\hline \multicolumn{2}{|r|}{torsion effusion} & \multicolumn{2}{|l|}{Knudsen effusion} & \multicolumn{2}{|l|}{transpiration-GC} \\
\hline t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa \\
\hline
\end{tabular}



FIGURE 4.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1-bromonaphthalene.

\subsection*{4.1.4.2 2-Bromonaphthalene}


Common Name: 2-Bromonaphthalene
Synonym: \(\beta\)-bromonaphthalene
Chemical Name: 2-bromonaphthalene
CAS Registry No: 580-13-2
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Br}\)
Molecular Weight: 207.067
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
55.9 (Lide 2003)

Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
281.5 (Lide 2003)

Density \(\left(\mathrm{g} / \mathrm{cm}^{3}\right.\) at \(\left.20^{\circ} \mathrm{C}\right)\) :
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
146.3 (Ruelle \& Kesselring 1997)
170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(\mathrm{pK}_{\mathrm{a}}\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
11.97 (Ruelle \& Kesselring 1997)

Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.498\left(\mathrm{mp}\right.\) at \(55.9^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) or as indicated):
\begin{tabular}{ll}
8.27 & (Yalkowsky et al. 1983) \\
7.72 & (calculated-molecular connectivity indices, Nirmalakhandan \& Speece 1989) \\
\(3.80,8.04\), & \(15.76\left(4,25,40^{\circ} \mathrm{C}\right.\), generator column-UV spec., Dickhut et al. 1994) \\
10.1 & (calculated-TSA, Dickhut et al. 1994) \\
9.04 & (calculated-group contribution method, Kühne et al. 1995) \\
8.06 & (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)
\end{tabular}

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations. Additional data at other temperatures designated \(*\) are compiled at the end of this section):
0.501* ( \(25.15^{\circ} \mathrm{C}\), solid I, transpiration method-GC, measured range 280.4-318.3 K, Verevkin 2003)
\(\ln \left(\mathrm{P} / \mathrm{P}^{0}\right)=314.110 / \mathrm{R}-94001.596 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(41.6 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\), where \(\mathrm{P}^{\mathrm{o}}=101.325 \mathrm{kPa}\), gas constant \(\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}\) (solid I , vapor pressure eq. from transpiration measurement, temp range 280.4-318.3 K, Verevkin 2003)
7.34* \(\quad\left(46.05^{\circ} \mathrm{C}\right.\), solid-II, transpiration method-GC, measured range 319.2-328.2 K, Verevkin 2003) \(\ln \left(\mathrm{P} / \mathrm{P}^{\mathrm{o}}\right)=302.672 / \mathrm{R}-90417.272 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(41.6 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\), where \(\mathrm{P}^{0}=101.325 \mathrm{kPa}\), gas constant \(\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}\) (solid II, vapor pressure eq. from transpiration measurements, temp range 319.2-328.2 K, Verevkin 2003)
18.75* ( \(57.05^{\circ} \mathrm{C}\), liquid, transpiration method-GC, measured range 330.2-360.2 K, Verevkin 2003)
\(\ln \left(\mathrm{P} / \mathrm{P}^{\circ}\right)=303.761 / \mathrm{R}-89574.863 / \mathrm{R} \cdot(\mathrm{T} / \mathrm{K})-(78.8 / \mathrm{R}) \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\), where \(\mathrm{P}^{\mathrm{o}}=101.325 \mathrm{kPa}\), gas constant \(\mathrm{R}=8.31451 \mathrm{~J} \cdot \mathrm{~K}^{-1} \cdot \mathrm{~mol}^{-1}\) (liquid, vapor pressure eq. from transpiration measurements, temp range 330.2-360.2 K, Verevkin 2003)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
4.35 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{oc}}\) :
Environmental Fate Rate Constants, k or Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\section*{TABLE 4.1.4.2.1}

Reported vapor pressures of 2-bromonaphthalene at various temperatures and the coefficients for the vapor pressure equations
\begin{tabular}{lll}
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})\) & \((1)\) & \(\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})\) \\
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\) & \((2)\) & \(\ln \mathrm{P}=\mathrm{A}-\mathrm{B} /\left(\mathrm{C}+\mathrm{t} /{ }^{\circ} \mathrm{C}\right)\) \\
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{C}+\mathrm{T} / \mathrm{K})\) & \((3)\) & \\
\(\log \mathrm{P}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \log (\mathrm{T} / \mathrm{K})\) & (4) & \(\ln \mathrm{P} / \mathrm{P}^{\mathrm{O}}=\mathrm{A}-\mathrm{B} /(\mathrm{T} / \mathrm{K})-\mathrm{C} \cdot \ln [(\mathrm{T} / \mathrm{K}) / 298.15]\)
\end{tabular}

Verevkin 2003
\begin{tabular}{|c|c|c|c|c|c|}
\hline \multicolumn{6}{|c|}{transpiration-GC} \\
\hline t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa & t/ \({ }^{\circ} \mathrm{C}\) & P/Pa \\
\hline \multicolumn{2}{|c|}{solid I} & \multicolumn{2}{|r|}{solid II} & \multicolumn{2}{|c|}{liquid} \\
\hline 7.25 & 0.105 & 46.05 & 77.34 & 57.05 & 18.75 \\
\hline 10.35 & 0.152 & 47.15 & 8.04 & 60.15 & 23.55 \\
\hline 15.15 & 0.287 & 48.05 & 8.68 & 63.15 & 28.58 \\
\hline 20.05 & 0.501 & 49.15 & 9.73 & 66.15 & 34.83 \\
\hline 25.05 & 0.886 & 51.05 & 11.47 & 69.15 & 41.76 \\
\hline 28.15 & 1.239 & 51.15 & 11.59 & 72.15 & 52.31 \\
\hline 31.15 & 1.709 & 53.15 & 13.60 & 75.15 & 61.76 \\
\hline 34.15 & 2.285 & 54.65 & 15.68 & 78.05 & 75.34 \\
\hline 37.15 & 3.107 & 55.05 & 16.20 & 81.05 & 88.25 \\
\hline 40.05 & 4.219 & & & 85.05 & 103.89 \\
\hline 41.15 & 4.588 & & & 87.05 & 125.40 \\
\hline 43.15 & 5.703 & & & & \\
\hline \multirow[t]{2}{*}{45.15} & \multirow[t]{2}{*}{6.686} & & & eq. 4 a & \(\mathrm{P} / \mathrm{kPa}\) \\
\hline & & eq. 4 a & \(\mathrm{P} / \mathrm{kPa}\) & \(\mathrm{P}^{0}\) & 101.325 kPa \\
\hline eq. 4 a & \(\mathrm{P} / \mathrm{kPa}\) & \(\mathrm{P}^{0}\) & 101.325 kPa & A & 303.761/R \\
\hline \(\mathrm{P}^{0}\) & 101.325 kPa & A & 302.672/R & B & 89574.863/R \\
\hline A & 314.110/R & B & 90417.272/R & C & 78.8/R \\
\hline B & 94001.596/R & C & 41.6/R & \multicolumn{2}{|l|}{\(\mathrm{R}=8.314 \mathrm{~J} \mathrm{~K}^{-1} \mathrm{~mol}^{-1}\)} \\
\hline C & 41.6/R & \multicolumn{2}{|l|}{\(\mathrm{R}=8.314 \mathrm{~J} \mathrm{~K}^{-1} \mathrm{~mol}^{-1}\)} & & \\
\hline \multicolumn{2}{|l|}{\multirow[t]{2}{*}{\(\mathrm{R}=8.314 \mathrm{~J} \mathrm{~K}^{-1} \mathrm{~mol}^{-1}\)}} & & & \multicolumn{2}{|l|}{\(\Delta \mathrm{H}_{\mathrm{V}} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=66.08\)} \\
\hline & & \multicolumn{2}{|l|}{\(\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=78.01\)} & & at 298.15 K \\
\hline \multicolumn{2}{|l|}{\(\Delta \mathrm{H}_{\text {subl }} /\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)=81.60\)} & \multicolumn{2}{|r|}{\multirow[t]{2}{*}{at 298.15 K}} & & \\
\hline \multicolumn{2}{|r|}{at 298.15 K} & & & & \\
\hline
\end{tabular}


FIGURE 4.1.4.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-bromonaphthalene.

\subsection*{4.1.4.3 1,4-Dibromonaphthalene}


Common Name: 1,4-Dibromonaphthalene
Synonym:
Chemical Name: 1,4-dibromonaphthalene
CAS Registry No: 83-53-4
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Br}_{2}\)
Molecular Weight: 285.963
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
83 (Lide 2003)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
310 (Lide 2003)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) at \(20^{\circ} \mathrm{C}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
194.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(\mathrm{pK}_{\mathrm{a}}\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.27\left(\mathrm{mp}\right.\) at \(83^{\circ} \mathrm{C}\) )
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) or as indicated):
\(0.125,0.35\), and \(0.866\left(4,25\right.\), and \(40^{\circ} \mathrm{C}\), generator column-GC/ECD, Dickhut et al. 1994)
1.92 (calculated-TSA, Dickhut et al. 1994)

Vapor Pressure \(\left(\mathrm{Pa}\right.\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k or Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.4.4 2,3-Dibromonaphthalene}


Common Name: 2,3-Dibromonaphthalene
Synonym:
Chemical Name: 2,3-dibromonaphthalene
CAS Registry No:
Molecular Formula: \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Br}_{2}\)
Molecular Weight: 285.963
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
140 (Lide 2003)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) at \(20^{\circ} \mathrm{C}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
194.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(\mathrm{pK}_{\mathrm{a}}\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.0744\left(\mathrm{mp}\right.\) at \(\left.140^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
\(0.0554,0.138\), and \(0.352\left(4,25\right.\), and \(40^{\circ} \mathrm{C}\), generator column-GC/ECD, Dickhut et al. 1994)
0.432 (calculated-TSA, Dickhut et al. 1994)

Vapor Pressure \(\left(\mathrm{Pa}\right.\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OW}}\) :
Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k or Half-Lives, \(\mathrm{t}_{1 / 2}\) :

Half-Lives in the Environment:

\subsection*{4.1.4.5 4-Bromobiphenyl}


Common Name: 4-Bromobiphenyl
Synonym:
Chemical Name: 4-bromobiphenyl
CAS Registry No: 92-66-0
Molecular Formula: \(\mathrm{C}_{12} \mathrm{H}_{.9} \mathrm{Br}\)
Molecular Weight: 233.103
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
91.5 (Lide 2003)

Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
310 (Weast 1983-84; Stephenson \& Malanowski 1987, Lide 2003)
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) at \(25^{\circ} \mathrm{C}\) ): 0.9327 (Weast 1983-84, Lide 2003)

Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
176.1 (Ruelle \& Kesselring 1997)
\(250.0 \quad\left(25^{\circ} \mathrm{C}\right.\), calculated-density)
207.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(\mathrm{pK}_{\mathrm{a}}\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) : 26.86 (Doucette \& Andren 1988)

Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.223\left(\mathrm{mp}\right.\) at \(91.5^{\circ} \mathrm{C}\) )
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations.):
\(0.235,0.653,0.874\left(4.9,25,40^{\circ} \mathrm{C}\right.\), generator column-GC, Doucette \& Andren 1988a)
\(\mathrm{S} /(\mathrm{mol} / \mathrm{L})=9.36 \times 10^{-7} \exp \left(0.037 \cdot \mathrm{t} /{ }^{\circ} \mathrm{C}\right)\) (generator column-GC/ECD, temp range \(4.9-40^{\circ} \mathrm{C}\), Doucette \& Andren 1988a); or \(\log x=-1436 /(\mathrm{T} / \mathrm{K})-1.541\), temp range \(4.9-40^{\circ} \mathrm{C}\) (generator column-GC/ECD, Doucette \& Andren 1988a) 0.546 (calculated-TSA, Dickhut et al. 1994)
0.256 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) and reported temperature dependence equations):
\(\log \left(\mathrm{P}_{\mathrm{L}} / \mathrm{kPa}\right)=2.24643-2174.97 /[(\mathrm{T} / \mathrm{K})-70.067]\); (Antoine eq., liquid state, temp range \(371-583 \mathrm{~K}\), Stephenson \& Malanowski 1987)

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{Ow}}\) :
4.96; 4.89, 5.00 (generator column-GC; calculated-group contribution method, estimated-TSA and \(\mathrm{K}_{\mathrm{OW}}\), Doucette \& Andren 1987) 4.96; 4.89, 4.83, 5.10, 5.14, 5.10 (generator column-GC; calculated- \(\pi\) const., HPLC-RT correlation, calculatedMW, calculated-MCI \(\chi\), calculated-TSA and \(\mathrm{K}_{\mathrm{ow}}\), Doucette \& Andren 1988b)
4.96 (recommended, Sangster 1993)
4.95 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k or Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.4.6 4,4'-Dibromobiphenyl}


Common Name: 4,4'-Dibromophenyl
Synonym: PBB-15, 4,4'-dibromo-1,1'-biphenyl
Chemical Name: 4,4'-dibromophenyl
CAS Registry No: 92-86-4
Molecular Formula: \(\mathrm{C}_{12} \mathrm{H}_{8} \mathrm{Br}_{2}\)
Molecular Weight: 312.000
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
164 (Ruelle \& Kesselring 1997, Lide 2003)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
357.5 (Lide 2003)

Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
192.2 (Ruelle \& Kesselring 1997)
231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: 0.0433 (mp at \(164^{\circ} \mathrm{C}\) )
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations):
0.00574 (generator column-GC, Gobas et al. 1988)
0.104 (quoted, Chessells et al. 1992)
\(0.0164 \quad\) (calculated-MCI \(\chi\), Ruelle \& Kesselring et al. 1997)
Vapor Pressure ( Pa at \(25^{\circ} \mathrm{C}\) ):
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\text {ow }}\) :
5.72; 5.75, 5.57 (generator column-GC; calculated-group contribution method, estimated-TSA and \(\mathrm{K}_{\mathrm{ow}}\), Doucette \& Andren 1987)
5.72; \(5.75,5.85,6.14,5.81,5.68\) (generator column-GC; calculated- \(\pi\) const., HPLC-RT correlation, calculatedMW, calculated-MCI \(\chi\), calculated-TSA and \(\mathrm{K}_{\text {OW }}\), Doucette \& Andren 1988b)
5.72 (HPLC-RT correlation, Gobas et al. 1988,)
5.72 (recommended, Sangster 1993)
4.67 (calculated-UNIFAC, Chen et al. 1993)
5.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
5.43 (guppy, lipid weight-based, Gobas et al. 1989)
4.19; 5.43 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)
3.825, 4.365 (calculated-MCI \(\chi, \mathrm{K}_{\mathrm{ow}}, \mathrm{Lu}\) et al. 1999)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\log \mathrm{k}_{1}=3.35 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
\(\log \mathrm{k}_{2}=-0.91 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:

\subsection*{4.1.4.7 2,4,6-Tribromobiphenyl}


Common Name: 2,4,6-Tribromobiphenyl
Synonym: PBB-30
Chemical Name: 2,4,6-tibromobiphenyl
CAS Registry No: 59080-33-0
Molecular Formula: \(\mathrm{C}_{12} \mathrm{H}_{7} \mathrm{Br}_{3}\)
Molecular Weight: 390.896
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
\(64 \quad\) (Ruelle \& Kesselring 1997)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
208.3 (Ruelle \& Kesselring 1997)
254.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.414\left(\mathrm{mp}\right.\) at \(\left.64^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.016 (generator column-GC, Gobas et al. 1988)
0.0131 (quoted, Chessells et al. 1992)
0.054 (calculated-MCI \(\chi\), Ruelle \& Kesselring 1997)

Vapor Pressure (Pa at \(25^{\circ} \mathrm{C}\) ):
Henry's Law Constant (Pa•m³/mol):
Octanol/Water Partition Coefficient, log \(\mathrm{K}_{\mathrm{ow}}\) :
6.03 (HPLC-RT correlation, Gobas et al. 1988, 1989)
6.03; 4.78 (quoted; calculated-UNIFAC, Chen et al. 1993)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
5.06 (guppy, lipid weight-based, Gobas et al. 1989)
3.97; 5.06 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)
4.408, 4.645 (calculated-MCI \(\chi, \mathrm{K}_{\mathrm{OW}}\), Lu et al. 1999)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\log \mathrm{k}_{1}=3.05 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-0.83 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:

\subsection*{4.1.4.8 2,2',5,5'-Tetrabromobiphenyl}


Common Name: 2, \(2^{\prime}, 5,5^{\prime}\)-Tetrabromobiphenyl
Synonym: PBB-52
Chemical Name: 2,2',5,5'-tetrabromobiphenyl
CAS Registry No: 59080-37-4
Molecular Formula: \(\mathrm{C}_{12} \mathrm{H}_{6} \mathrm{Br}_{4}\)
Molecular Weight: 469.792
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
144 (Ruelle \& Kesselring 1997)
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
224.4 (Ruelle \& Kesselring 1997)
277.8 (calculated-Le Bas at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\left.\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\right), \mathrm{F}: 0.068\left(\mathrm{mp}\right.\) at \(\left.144^{\circ} \mathrm{C}\right)\)
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
0.00429 (generator column-GC, Gobas et al. 1988)
0.0545 (quoted, Chessells et al. 1992)
0.00409 (calculated-AQUAFAC, Myrdal et al. 1995)
0.00246 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)

Vapor Pressure \(\left(\mathrm{Pa}\right.\) at \(\left.25^{\circ} \mathrm{C}\right)\) :

Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, log \(\mathrm{K}_{\mathrm{Ow}}\) :
6.50 (HPLC-RT correlation, Gobas et al. 1988,)
4.88 (calculated-UNIFAC group contribution, Chen et al. 1993)

Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
6.16 (guppy, lipid weight-based, Gobas et al. 1989)
4.62; 6.16 (flowing water system-whole weight of fish; lipid content, quoted, Lu et al. 1999)
5.097; 6.16 (calculated-MCI \(\chi, \mathrm{K}_{\mathrm{ow}}\), Lu et al. 1999)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\log \mathrm{k}_{1}=2.96 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-2.02 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:

\subsection*{4.1.4.9 2,2',4,5,5'-Pentabromobiphenyl}


Common Name: 2,2',4,5,5'-Pentabromobiphenyl
Synonym:
Chemical Name: \(2,2^{\prime}, 4,5,5^{\prime}\)-pentabromobiphenyl
CAS Registry No: 6788-96-4
Molecular Formula: \(\mathrm{C}_{12} \mathrm{H}_{5} \mathrm{Br}_{5}\)
Molecular Weight: 548.688
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
157 (Dickhut et al. 1994; Ruelle \& Kesselring 1997)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density \(\left(\mathrm{g} / \mathrm{cm}^{3}\right.\) at \(\left.20^{\circ} \mathrm{C}\right)\) :
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
301.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant \(\mathrm{pK}_{\mathrm{a}}\) :
Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
45.44 (Doucette \& Andren 1988)

Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: \(0.0507\left(\mathrm{mp}\right.\) at \(157^{\circ} \mathrm{C}\) )

Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) or as indicated and reported temperature dependence equations.): \(1.032 \times 10^{-4}, 4.42 \times 10^{-4}, 9.82 \times 10^{-4}\left(4.9,25,40^{\circ} \mathrm{C}\right.\), generator column-GC/ECD, Doucette \& Andren 1988a) \(\mathrm{S} /(\mathrm{mol} / \mathrm{L})=1.52 \times 10^{-10} \exp \left(0.063 \cdot \mathrm{t}^{\circ} \mathrm{C}\right)\) (generator column-GC, temp range \(4-40^{\circ} \mathrm{C}\), Doucette \& Andren 1988a) \(\log x=-2374 /(\mathrm{T} / \mathrm{K})-2.373\), temp range \(4-40^{\circ} \mathrm{C}\) (generator column-GC, Doucette \& Andren 1988a)

Vapor Pressure (Pa at \(25^{\circ} \mathrm{C}\) ):
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\text {ow }}\) :
77.10 (generator column-GC Doucette \& Andren 1987)
77.10; 8.76 (generator column-GC; HPLC-RT correlation, Doucette \& Andren 1988b)
7.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{oc}}\) :
Environmental Fate Rate Constants, \(k\) or Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.1.4.10 2,2', 4, \(\mathbf{4}^{\prime}, \mathbf{6}, \mathbf{6}^{\prime}\)-Hexabromobiphenyl}


Common Name: 2,2',4,4',6,6'-Hexabromobiphenyl
Synonym: 2,2',4,4',6,6'-HBB
Chemical Name: \(2,2^{\prime}, 4,4^{\prime}, 6,6^{\prime}\)-hexabromobiphenyl
CAS Registry No: 59261-08-4
Molecular Formula: \(\mathrm{C}_{22} \mathrm{H}_{4} \mathrm{Br}_{6}\)
Molecular Weight: 627.584
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
176 (Gobas et al. 1988; Ruelle \& Kesselring 1997)
Boiling Point \(\left({ }^{\circ} \mathrm{C}\right)\) :
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
256.6 (Ruelle \& Kesselring 1997)
324.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F: 0.033 (mp at \(176^{\circ} \mathrm{C}\) )
Water Solubility ( \(\mathrm{g} / \mathrm{m}^{3}\) or \(\mathrm{mg} / \mathrm{L}\) at \(25^{\circ} \mathrm{C}\) ):
\(6.23 \times 10^{-4}\) (generator column-GC, Gobas et al. 1988)
0.0210 (lit. mean, Chessells et al. 1992)
\(1.04 \times 10^{-4}\) (calculated-molar volume, mp and mobile order thermodynamics, Ruelle \& Kesselring 1997)
Vapor Pressure (Pa at \(25^{\circ} \mathrm{C}\) ):
\(8.033 \times 10^{-6}\) (for hexabrominated biphenyl, GC-RT correlation, Watanabe \& Tatsukawa 1989)
\(4.52 \times 10^{-10}\) (quoted, Pijnenburg et al. 1995)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{ow}}\) :
7.50 (for hexabrominated biphenyl, reversed phase-HPLC-RT correlation, Watanabe \& Tatsukawa 1989)
7.20 (HPLC-RT correlation, Gobas et al. 1987, 1989)
7.20; 5.09 (quoted; calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log \mathrm{BCF}\) or \(\log \mathrm{K}_{\mathrm{B}}\) :
5.85 (guppy, lipid weight-based, Gobas et al. 1989)
4.26 (calculated-K \(\mathrm{K}_{\text {ow }}\), Chessells et al. 1992)

Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{oc}}\) :
Environmental Fate Rate Constants, k and Half-Lives, \(\mathrm{t}_{1 / 2}\) :
Bioconcentration and Uptake and Elimination Rate Constants ( \(\mathrm{k}_{1}\) and \(\mathrm{k}_{2}\) ):
\(\log \mathrm{k}_{1}=2.51 \mathrm{~d}^{-1} ; \log \mathrm{k}_{2}=-2.15 \mathrm{~d}^{-1}\) (guppy, Gobas et al. 1989)
Half-Lives in the Environment:

\subsection*{4.1.4.11 Decabromobiphenyl}


Common Name: Decabromobiphenyl
Synonym: PBB-209
Chemical Name:
CAS Registry No: 13654-09-6
Molecular Formula: \(\mathrm{C}_{12} \mathrm{Br}_{10}\)
Molecular Weight: 943.168
Melting Point ( \({ }^{\circ} \mathrm{C}\) ):
Boiling Point ( \({ }^{\circ} \mathrm{C}\) ):
Density ( \(\mathrm{g} / \mathrm{cm}^{3}\) ):
Molar Volume ( \(\mathrm{cm}^{3} / \mathrm{mol}\) ):
417.6 (calculated-Le Bas method at normal boiling point)

Heat of Fusion, \(\Delta \mathrm{H}_{\text {fus }}(\mathrm{kJ} / \mathrm{mol})\) :
Entropy of Fusion, \(\Delta \mathrm{S}_{\text {fus }}(\mathrm{J} / \mathrm{mol} \mathrm{K})\) :
Fugacity Ratio at \(25^{\circ} \mathrm{C}\) (assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\) ), F :
Water Solubility \(\left(\mathrm{g} / \mathrm{m}^{3}\right.\) or \(\mathrm{mg} / \mathrm{L}\) at \(\left.25^{\circ} \mathrm{C}\right)\) :
Vapor Pressure (Pa at \(25^{\circ} \mathrm{C}\) ):
\(>1.33 \times 10^{-9} \quad(\) GC-RT correlation, Watanabe \& Tatsukawa 1989)
\(<7.4 \times 10^{-4} \quad\) (quoted, Pijnenburg et al. 1995)
Henry's Law Constant ( \(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\) ):
Octanol/Water Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OW}}\) :
8.58; 12.63, 9.36 (generator column-GC; calculated-group contribution method, estimated-TSA and \(\mathrm{K}_{\mathrm{ow}}\), Doucette \& Andren 1987)
\(8.58 ; 10.42,13.87,8.46,8.69,7.10\) (generator column-GC; calculated- \(\pi\) const., HPLC-RT correlation, calculated-
MW, calculated-MCI \(\chi\), calculated-TSA and K
8.60 (reversed phase-HPLC-RT correlation, Watanabe \& Tatsukawa 1989)

Octanol/Air Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OA}}\) :
Bioconcentration Factor, \(\log\) BCF or \(\log K_{B}\) :
Sorption Partition Coefficient, \(\log \mathrm{K}_{\mathrm{OC}}\) :
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1 / 2}\) :
Half-Lives in the Environment:

\subsection*{4.2 SUMMARY TABLES AND QSPR PLOTS}

TABLE 4.2.1
Summary of physical properties of polynuclear aromatic hydrocarbons (PAHs)
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline \multirow[b]{2}{*}{Compound} & \multirow[b]{2}{*}{CAS no.} & \multirow[b]{2}{*}{Molecular formula} & \multirow[t]{2}{*}{Molecular weight, MW \(\mathrm{g} / \mathrm{mol}\)} & \multirow[b]{2}{*}{m.p. \({ }^{\circ} \mathrm{C}\)} & \multirow[b]{2}{*}{b.p. \({ }^{\circ} \mathrm{C}\)} & \multirow[b]{2}{*}{Fugacity ratio, F at \(\mathbf{2 5}^{\circ} \mathrm{C}^{*}\)} & \multicolumn{2}{|l|}{Molar volume, \(\mathrm{V}_{\mathrm{M}} \mathrm{cm}^{3} / \mathrm{mol}\)} \\
\hline & & & & & & & MW/ \(/\) at \(\mathbf{2 0}^{\circ} \mathrm{C}\) & Le Bas \\
\hline Indan & 496-11-7 & \(\mathrm{C}_{9} \mathrm{H}_{10}\) & 118.175 & -51.38 & 177.97 & 1 & 123.0 & 143.7 \\
\hline Naphthalene & 91-20-3 & \(\mathrm{C}_{10} \mathrm{H}_{8}\) & 128.171 & 80.26 & 217.9 & 0.287 & 125.0 & 147.6 \\
\hline 1-Methyl- & 90-12-0 & \(\mathrm{C}_{11} \mathrm{H}_{10}\) & 142.197 & -30.43 & 244.7 & 1 & 139.4 & 169.8 \\
\hline 2-Methyl- & 91-57-6 & \(\mathrm{C}_{11} \mathrm{H}_{10}\) & 142.197 & 34.6 & 241.1 & 0.805 & 141.4 & 169.8 \\
\hline 1,2-Dimethyl- & 573-98-8 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & 0.8 & 266.5 & 1 & & 192.0 \\
\hline 1,3-Dimethyl- & 575-41-7 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & -6 & 263 & 1 & 154.0 & 192.0 \\
\hline 1,4-Dimethyl- & 571-58-4 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & 7.6 & 268 & 1 & 153.7 & 192.0 \\
\hline 1,5-Dimethyl- & 571-61-9 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & 82 & 265 & 0.276 & & 192.0 \\
\hline 2,3-Dimethyl- & 581-40-8 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & 105 & 268 & 0.164 & 155.8 & 192.0 \\
\hline 2,6-Dimethyl- & 581-42-0 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & 112 & 262 & 0.140 & 155.8 & 192.0 \\
\hline 1-Ethyl- & 1127-76-0 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & -10.9 & 258.6 & 1 & 155.0 & 192.0 \\
\hline 2-Ethyl- & 939-27-5 & \(\mathrm{C}_{12} \mathrm{H}_{12}\) & 156.223 & -7.4 & 258 & 1 & 157.4 & 192.0 \\
\hline 1,4,5-Trimethyl- & 2131-41-1 & \(\mathrm{C}_{13} \mathrm{H}_{14}\) & 170.250 & 63 & 285 & 0.424 & & 214.2 \\
\hline Biphenyl & 92-52-4 & \(\mathrm{C}_{12} \mathrm{H}_{10}\) & 154.207 & 68.93 & 256.1 & 0.371 & 148.3 & 184.6 \\
\hline 4-Methyl- & 644-08-6 & \(\mathrm{C}_{13} \mathrm{H}_{12}\) & 168.234 & 49.5 & 267.5 & 0.575 & & 206.8 \\
\hline 4,4'-Dimethyl- & 613-33-2 & \(\mathrm{C}_{14} \mathrm{H}_{14}\) & 182.261 & 125 & 295 & 0.104 & & 229.0 \\
\hline Diphenylmethane & 101-81-5 & \(\mathrm{C}_{13} \mathrm{H}_{12}\) & 168.234 & 25.4 & 265 & 0.991 & 167.2 & 206.8 \\
\hline Bibenzyl & 103-29-7 & \(\mathrm{C}_{14} \mathrm{H}_{14}\) & 182.261 & 52.5 & 284 & 0.537 & & 229.0 \\
\hline trans-Stilbene & 103-30-0 & \(\mathrm{C}_{14} \mathrm{H}_{12}\) & 180.245 & 124.2 & 307 & 0.106 & 185.7 & 221.6 \\
\hline Acenaphthylene & 208-96-8 & \(\mathrm{C}_{12} \mathrm{H}_{8}\) & 150.192 & 91.8 & 280 & 0.221 & & 165.7 \\
\hline Acenaphthene & 83-32-9 & \(\mathrm{C}_{12} \mathrm{H}_{10}\) & 154.207 & 93.4 & 279 & 0.213 & 126.2 & 173.1 \\
\hline Fluorene & 86-73-7 & \(\mathrm{C}_{13} \mathrm{H}_{10}\) & 166.218 & 114.77 & 295 & 0.132 & & 187.9 \\
\hline 1-Methylfluorene & 1730-37-6 & \(\mathrm{C}_{14} \mathrm{H}_{12}\) & 180.245 & 87 & 318 & 0.246 & & 210.1 \\
\hline Phenanthrene & 85-01-8 & \(\mathrm{C}_{14} \mathrm{H}_{10}\) & 178.229 & 99.24 & 340 & 0.187 & & 199.2 \\
\hline 1-Methyl- & 832-69-9 & \(\mathrm{C}_{15} \mathrm{H}_{12}\) & 192.256 & 123 & 354 & 0.109 & & 221.4 \\
\hline Anthracene & 120-12-7 & \(\mathrm{C}_{14} \mathrm{H}_{10}\) & 178.229 & 215.76 & 339.9 & 0.0134 & & 196.7 \\
\hline 2-Methyl- & 613-12-7 & \(\mathrm{C}_{15} \mathrm{H}_{12}\) & 192.256 & 209 & 359 & 0.0157 & & 218.9 \\
\hline 9-Methyl- & 779-02-2 & \(\mathrm{C}_{15} \mathrm{H}_{12}\) & 192.256 & 81.5 & & 0.279 & & 218.9 \\
\hline 9,10-Dimethyl- & 781-43-1 & \(\mathrm{C}_{16} \mathrm{H}_{14}\) & 206.282 & 183.6 & 360 & 0.0278 & & 241.1 \\
\hline
\end{tabular}
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline \multirow[b]{2}{*}{Compound} & \multirow[b]{2}{*}{CAS no.} & \multirow[b]{2}{*}{Molecular formula} & \multirow[t]{2}{*}{Molecular weight, MW \(\mathrm{g} / \mathrm{mol}\)} & \multirow[b]{2}{*}{m.p. \({ }^{\circ} \mathrm{C}\)} & \multirow[b]{2}{*}{b.p. \({ }^{\circ} \mathrm{C}\)} & \multirow[b]{2}{*}{Fugacity ratio, F at \(25^{\circ} \mathrm{C}^{*}\)} & \multicolumn{2}{|l|}{Molar volume, \(\mathrm{V}_{\mathrm{M}} \mathrm{cm}^{3} / \mathrm{mol}\)} \\
\hline & & & & & & & MW/ \(/\) at \(20^{\circ} \mathrm{C}\) & Le Bas \\
\hline Pyrene & 129-00-0 & \(\mathrm{C}_{16} \mathrm{H}_{10}\) & 202.250 & 150.62 & 404 & 0.0585 & & 213.8 \\
\hline Fluoranthene & 206-44-0 & \(\mathrm{C}_{16} \mathrm{H}_{10}\) & 202.250 & 110.19 & 384 & 0.146 & & 217.3 \\
\hline Benzo[a]fluorene & 238-84-6 & \(\mathrm{C}_{17} \mathrm{H}_{12}\) & 216.227 & 189.5 & 405 & 0.0243 & & 239.5 \\
\hline Benzo[b]fluorene & 243-17-4 & \(\mathrm{C}_{17} \mathrm{H}_{12}\) & 216.227 & 212 & 401 & 0.0146 & & 239.5 \\
\hline Chrysene & 218-01-9 & \(\mathrm{C}_{18} \mathrm{H}_{12}\) & 228.288 & 255.5 & 448 & 0.00548 & 179.2 & 250.8 \\
\hline Triphenylene & 217-59-4 & \(\mathrm{C}_{18} \mathrm{H}_{12}\) & 228.288 & 197.8 & 425 & 0.0202 & & 250.8 \\
\hline \(o\)-Terphenyl & 84-15-1 & \(\mathrm{C}_{18} \mathrm{H}_{14}\) & 230.304 & 56.2 & 332 & 0.494 & & 273.2 \\
\hline \(m\)-Terphenyl & 92-06-8 & \(\mathrm{C}_{18} \mathrm{H}_{14}\) & 230.304 & 87 & 363 & 0.246 & 192.1 & 273.2 \\
\hline \(p\)-Terphenyl & 92-94-4 & \(\mathrm{C}_{18} \mathrm{H}_{14}\) & 230.304 & 213.9 & 376 & 0.0140 & & 273.2 \\
\hline Naphthacene & 92-24-0 & \(\mathrm{C}_{18} \mathrm{H}_{12}\) & 228.288 & 357 & sublim & 0.00055 & & 250.8 \\
\hline Benz[a]anthracene & 56-55-3 & \(\mathrm{C}_{18} \mathrm{H}_{12}\) & 228.288 & 160.5 & 438 & 0.0468 & & 248.3 \\
\hline Benzo[b]fluoranthene & 205-99-2 & \(\mathrm{C}_{20} \mathrm{H}_{12}\) & 252.309 & 168 & 481 & 0.0395 & & 268.9 \\
\hline Benzo[j]fluoranthene & 205-82-3 & \(\mathrm{C}_{20} \mathrm{H}_{12}\) & 252.309 & 166 & 480 & 0.0414 & & 268.9 \\
\hline Benzo[ \(k\) ]fluoranthene & 207-08-9 & \(\mathrm{C}_{20} \mathrm{H}_{12}\) & 252.309 & 217 & 480 & 0.0131 & & 268.9 \\
\hline Benzo[a]pyrene & 50-32-8 & \(\mathrm{C}_{20} \mathrm{H}_{12}\) & 252.309 & 181.1 & 495 & 0.0294 & & 262.9 \\
\hline Benzo[e]pyrene & 192-97-2 & \(\mathrm{C}_{20} \mathrm{H}_{12}\) & 252.309 & 181.4 & 311 & 0.0292 & & 262.9 \\
\hline Perylene & 198-55-0 & \(\mathrm{C}_{20} \mathrm{H}_{12}\) & 252.309 & 277.76 & 503 & 0.00331 & & 262.9 \\
\hline 7,12-DMBA & 57-97-6 & \(\mathrm{C}_{20} \mathrm{H}_{16}\) & 256.341 & 122.5 & & 0.111 & & 292.7 \\
\hline 9,10-DMBA & 56-56-35 & \(\mathrm{C}_{20} \mathrm{H}_{16}\) & 256.341 & 122 & & 0.112 & & 292.7 \\
\hline 3-MCA & 56-49-5 & \(\mathrm{C}_{21} \mathrm{H}_{16}\) & 268.352 & 180 & & 0.0301 & 209.6 & 296.0 \\
\hline Benzo[ghi]perylene & 191-24-2 & \(\mathrm{C}_{22} \mathrm{H}_{12}\) & 276.330 & 272.5 & & 0.00373 & & 277.5 \\
\hline Indeno[1,2,3-c,d]pyrene & 193-39-5 & \(\mathrm{C}_{22} \mathrm{H}_{12}\) & 276.330 & 162 & & 0.0453 & & 283.5 \\
\hline Dibenz[ \(a, c\) ]anthracene & 215-58-7 & \(\mathrm{C}_{22} \mathrm{H}_{14}\) & 278.346 & 205 & & 0.0171 & & 299.9 \\
\hline Dibenz \([a, h]\) anthracene & 53-70-3 & \(\mathrm{C}_{22} \mathrm{H}_{14}\) & 278.346 & 269.5 & 524 & 0.00399 & & 299.9 \\
\hline Dibenz[ \(a, j\) ]anthracene & 224-41-9 & \(\mathrm{C}_{22} \mathrm{H}_{14}\) & 278.346 & 197.5 & & 0.0203 & & 299.9 \\
\hline Pentacene & 135-48-8 & \(\mathrm{C}_{22} \mathrm{H}_{14}\) & 278.346 & > 300 dec & & & & 299.9 \\
\hline Coronene & 191-07-1 & \(\mathrm{C}_{24} \mathrm{H}_{12}\) & 300.352 & 437.4 & 525 & 0.00009 & & 292.1 \\
\hline 2,4",5-Trichloro-p-terphenyl & 61576-93-0 & \(\mathrm{C}_{18} \mathrm{H}_{11} \mathrm{Cl}_{3}\) & 333.639 & 92 & & 0.220 & & 335.9 \\
\hline 2,4,4",6-Tetrachloro-p-terphenyl & & \(\mathrm{C}_{18} \mathrm{H}_{10} \mathrm{Cl}_{4}\) & 368.084 & 114 & & 0.134 & & 356.8 \\
\hline 1-Chloronaphthalene & 90-13-1 & \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Cl}\) & 162.616 & -2.5 & 259 & 1 & 136.2 & 168.5 \\
\hline 2-Chloronaphthalene & 91-58-7 & \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Cl}\) & 162.616 & 58 & 256 & 0.474 & & 168.5 \\
\hline 1,2-Dichloronaphthalene & 2050-69-3 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\) & 197.061 & 36 & 296.5 & 0.780 & & 189.4 \\
\hline 1,4-Dichloronaphthalene & 1825-31-6 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\) & 197.061 & 67.5 & 288 & 0.383 & & 189.4 \\
\hline 1,8-Dichloronaphthalene & 2050-74-0 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\) & 197.061 & 89 & sublim & 0.236 & & 189.4 \\
\hline
\end{tabular}
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline 2,3-Dichloronaphthalene & 2050-75-1 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\) & 197.061 & 120 & & 0.117 & & 189.4 \\
\hline 2,7-Dichloronaphthalene & 2198-77-8 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Cl}_{2}\) & 197.061 & 115 & & 0.131 & & 189.4 \\
\hline 1,2,3-Trichloronaphthalene & 50402-52-3 & \(\mathrm{C}_{10} \mathrm{H}_{5} \mathrm{Cl}_{3}\) & 231.506 & 81-84 & & 0.273 & & 210.3 \\
\hline 1,3,7-Trichloronaphthalene & 55720-37-1 & \(\mathrm{C}_{10} \mathrm{H}_{5} \mathrm{Cl}_{3}\) & 231.506 & 113 & 274 & 0.137 & & 210.3 \\
\hline 1,2,3,4-Tetrachloronaphthalene & 20020-02-4 & \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\) & 265.951 & 199 & & 0.0196 & & 231.2 \\
\hline 1,2,3,5-Tetrachloronaphthalene & 53555-63-8 & \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\) & 265.951 & 141 & & 0.0728 & & 231.2 \\
\hline 1,3,5,7-Tetrachloronaphthalene & 53555-64-9 & \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\) & 265.951 & 179 & & 0.0308 & & 231.2 \\
\hline 1,3,5,8-Tetrachloronaphthalene & 31604-28-1 & \(\mathrm{C}_{10} \mathrm{H}_{4} \mathrm{Cl}_{4}\) & 265.951 & 131 & & 0.0912 & & 231.2 \\
\hline 1,2,3,4,6-Pentachloronaphthalene & 67922-25-2 & \(\mathrm{C}_{10} \mathrm{H}_{3} \mathrm{Cl}_{5}\) & 300.396 & 147 & & 0.0635 & & 252.1 \\
\hline 1,2,3,5,7-Pentachloronaphthalene & 53555-65-0 & \(\mathrm{C}_{10} \mathrm{H}_{3} \mathrm{Cl}_{5}\) & 300.396 & 171 & 313 & 0.0369 & & 252.1 \\
\hline 1,2,3,5,8-Pentachloronaphthalene & 150224-24-1 & \(\mathrm{C}_{10} \mathrm{H}_{3} \mathrm{Cl}_{5}\) & 300.396 & 174-176 & & 0.0340 & & 252.1 \\
\hline 1,2,3,4,5,7-Hexachloronaphthalene & 67927-67-4 & \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\) & 334.842 & 194 & 331 & 0.0220 & & 273.0 \\
\hline 1,2,3,4,6,7-Hexachloronaphthalene & 103426-96-6 & \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\) & 334.842 & 205-206 & & 0.0340 & & 273.0 \\
\hline 1,2,3,5,6,7-Hexachloronaphthalene & 103426-97-7 & \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\) & 334.842 & 234-235 & & 0.00880 & & 273.0 \\
\hline 1,2,3,5,7,8-Hexachloronaphthalene & 103426-94-4 & \(\mathrm{C}_{10} \mathrm{H}_{2} \mathrm{Cl}_{6}\) & 334.842 & 148-149 & & 0.0614 & & 273.0 \\
\hline 1,2,3,4,5,6,7-Heptachloro- & 58863-14-2 & \(\mathrm{C}_{10} \mathrm{HCl}_{7}\) & 369.287 & & & & & 293.9 \\
\hline 1,2,3,4,5,6,8-Heptachloro- & 58863-15-3 & \(\mathrm{C}_{10} \mathrm{HCl}_{7}\) & 369.287 & 194 & 348 & 0.0220 & & 293.9 \\
\hline Octachloronaphthalene & 2234-13-1 & \(\mathrm{C}_{10} \mathrm{Cl}_{8}\) & 403.731 & 197.5 & 365 & 0.0203 & & 314.8 \\
\hline 1-Bromonaphthalene & 90-11-9 & \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Br}\) & 207.067 & 6.1 & 281 & 1 & 140.0 & 170.9 \\
\hline 2-Bromonaphthalene & 580-13-1 & \(\mathrm{C}_{10} \mathrm{H}_{7} \mathrm{Br}\) & 207.067 & 55.9 & 281.5 & 0.498 & & 170.9 \\
\hline 1,4-Dibromonaphthalene & 83-53-4 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Br}_{2}\) & 285.963 & 83 & 310 & 0.270 & & 194.2 \\
\hline 2,3-Dibromonaphthalene & 13214-70-5 & \(\mathrm{C}_{10} \mathrm{H}_{6} \mathrm{Br}_{2}\) & 285.963 & 140 & & 0.0744 & & 194.2 \\
\hline 4-Bromobiphenyl & 92-66-0 & \(\mathrm{C}_{12} \mathrm{H}_{9} \mathrm{Br}\) & 233.103 & 91.5 & 310 & 0.223 & & 207.9 \\
\hline 4,4'-Dibromobiphenyl & 92-86-4 & \(\mathrm{C}_{12} \mathrm{H}_{8} \mathrm{Br}_{2}\) & 312.000 & 164 & 357.5 & 0.0433 & & 231.2 \\
\hline 2,4,6-Tribromobiphenyl & 59080-33-0 & \(\mathrm{C}_{12} \mathrm{H}_{7} \mathrm{Br}_{3}\) & 390.896 & 64 & & 0.414 & & 254.5 \\
\hline 2,2',5,5'-Tetrabromobiphenyl & 59080-37-4 & \(\mathrm{C}_{12} \mathrm{H}_{6} \mathrm{Br}_{4}\) & 469.792 & 144 & & 0.0680 & & 277.8 \\
\hline 2,2',4,5,5'-Pentabromobiphenyl & 6788-96-4 & \(\mathrm{C}_{12} \mathrm{H}_{5} \mathrm{Br}_{5}\) & 548.688 & 157 & & 0.0507 & & 301.1 \\
\hline 2,2',4,4',6,6'-Hexabromobiphenyl & 59261-08-4 & \(\mathrm{C}_{12} \mathrm{H}_{4} \mathrm{Br}_{6}\) & 627.584 & 176 & & 0.0330 & & 324.4 \\
\hline Decabromobiphenyl & 13654-09-6 & \(\mathrm{C}_{12} \mathrm{Br}_{10}\) & 943.168 & & & & & 417.6 \\
\hline
\end{tabular}

Note:
\begin{tabular}{ll} 
3-MCA & 3-Methylcholanthrene \\
7,12-DMBA & 7,12-Dimethylbenz \([a]\) anthracene \\
\(9,10-\mathrm{DMBA}\) & 9,10-Dimethylbenz[ \(a\) anthracene
\end{tabular}
* Assuming \(\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}\).

7,12-Dimethylbenz[a]anthracene
9,10-Dimethylbenz[a]anthracene

TABLE 4.2.2
Summary of selected physical-chemical properties of polynuclear aromatic hydrocarbons (PAHs) at \(25^{\circ} \mathrm{C}\)
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline \multirow[b]{3}{*}{Compund} & \multicolumn{2}{|l|}{Selected properties} & \multicolumn{3}{|c|}{\multirow[b]{2}{*}{Solubility}} & \multirow[b]{3}{*}{\(\boldsymbol{\operatorname { l o g }} \mathrm{K}_{\text {Ow }}\)} & \multirow[t]{3}{*}{Henry's law constant \(\mathrm{H} /\left(\mathrm{Pa} \cdot \mathrm{m}^{3} / \mathrm{mol}\right)\) calculated P/C} \\
\hline & \multicolumn{2}{|l|}{Vapor pressure} & & & & & \\
\hline & Ps/Pa & \(\mathbf{P}_{\mathbf{L}} / \mathbf{P a}\) & \(\mathbf{S} /\left(\mathrm{g} / \mathrm{m}^{3}\right)\) & \(\mathrm{C}^{\mathrm{S}} /\left(\mathrm{mmol} / \mathrm{m}^{3}\right)\) & \(\mathrm{C}_{\mathrm{L}} /\left(\mathrm{mmol} / \mathrm{m}^{3}\right)\) & & \\
\hline Indan & 197 & 197 & 100 & 846.2 & 846.2 & 3.33 & 232.8 \\
\hline Naphthalene & 10.4 & 36.24 & 31 & 241.9 & 842.7 & 3.37 & 43.00 \\
\hline 1-Methyl- & 8.84 & 8.84 & 28 & 196.9 & 196.9 & 3.87 & 44.89 \\
\hline 2-Methyl- & 9.0 & 11.2 & 25 & 175.8 & 218.4 & 3.86 & 51.19 \\
\hline 1,2-Dimethyl- & 0.87 & 0.87 & & & & 4.31 & \\
\hline 1,3-Dimethyl- & & & 8 & 51.21 & 51.21 & 4.42 & \\
\hline 1,4-Dimethyl- & 2.27 & 2.27 & 11.4 & 72.97 & 72.97 & 4.37 & 31.11 \\
\hline 1,5-Dimethyl- & & & 3.1 & 19.84 & 71.90 & 4.38 & \\
\hline 2,3-Dimethyl- & 1.0 & 6.10 & 2.5 & 16.00 & 97.58 & 4.40 & 62.49 \\
\hline 2,6-Dimethyl- & 1.4 & 10.0 & 1.7 & 10.88 & 77.73 & 4.31 & 128.7 \\
\hline 1-Ethyl- & 2.51 & 2.51 & 10.1 & 64.65 & 64.65 & 4.40 & 38.82 \\
\hline 2-Ethyl- & 4.0 & 4.0 & 8.0 & 51.21 & 51.21 & 4.38 & 78.11 \\
\hline 1,4,5-Trimethyl- & 0.681 & 1.61 & 2.1 & 12.33 & 29.09 & 5.00 & 55.21 \\
\hline Biphenyl & 1.3 & 3.50 & 7.0 & 45.39 & 122.4 & 3.90 & 28.64 \\
\hline 4-Methyl- & & & 4.05 & 24.07 & 41.87 & 4.63 & \\
\hline 4,4'-Dimethyl- & & & 0.175 & 0.960 & 9.232 & 5.09 & \\
\hline Diphenylmethane & 0.0885 & 0.0893 & 16 & 95.10 & 95.10 & 4.14 & 0.931 \\
\hline Bibenzyl & 0.406 & 0.756 & 4.37 & 23.98 & 44.65 & 4.70 & 16.93 \\
\hline trans-Stilbene & 0.065 & 0.613 & 0.29 & 1.609 & 15.18 & 4.81 & 40.40 \\
\hline Acenaphthylene & 0.9 & 4.14 & 16.1 & 107.2 & 485.0 & 4.00 & 8.396 \\
\hline Acenaphthene & 0.3 & 1.41 & 3.80 & 24.64 & 115.7 & 3.92 & 12.17 \\
\hline Fluorene & 0.09 & 0.682 & 1.90 & 11.43 & 85.60 & 4.18 & 7.873 \\
\hline 1-Methyl- & & & 1.09 & 6.047 & 24.58 & 4.97 & \\
\hline Phenanthrene & 0.02 & 0.107 & 1.10 & 6.172 & 33.00 & 4.57 & 3.240 \\
\hline 1-Methyl- & & & 0.27 & 1.404 & 12.88 & 5.14 & \\
\hline Anthracene & 0.001 & 0.0746 & 0.045 & 0.252 & 18.84 & 4.54 & 3.961 \\
\hline 2-Methyl- & & & 0.03 & 0.156 & 9.939 & 5.15 & \\
\hline 9-Methyl- & 0.00224 & 0.00803 & 0.261 & 1.358 & 4.866 & 5.07 & 1.650 \\
\hline 9,10-Dimethyl- & \(1.53 \times 10^{-4}\) & \(5.50 \times 10^{-3}\) & 0.056 & 0.271 & 9.765 & 5.25 & 0.564 \\
\hline Pyrene & 0.0006 & 0.0119 & 0.132 & 0.652 & 12.89 & 5.18 & 0.919 \\
\hline Fluoranthene & 0.00123 & \(8.42 \times 10^{-3}\) & 0.26 & 1.286 & 8.805 & 5.22 & 0.957 \\
\hline Benzo[ \(a\) ]fluorene & & & 0.045 & 0.208 & 8.564 & 5.40 & \\
\hline
\end{tabular}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline Benzo[b]fluorene & & & 0.002 & 0.00925 & 0.634 & 5.75 & \\
\hline Chrysene & \(5.70 \times 10^{-7}\) & \(1.07 \times 10^{-4}\) & 0.002 & 0.00876 & 1.599 & 5.60 & 0.065 \\
\hline Triphenylene & \(2.30 \times 10^{-9}\) & \(1.21 \times 10^{-4}\) & 0.043 & 0.188 & 9.325 & 5.49 & 0.012 \\
\hline \(p\)-Terphenyl & \(4.86 \times 10^{-9}\) & \(3.47 \times 10^{-4}\) & 0.0180 & 0.0782 & 5.583 & 6.03 & 0.062 \\
\hline Naphthacene & \(7.30 \times 10^{-9}\) & \(1.33 \times 10^{-5}\) & 0.0006 & 0.00263 & 4.779 & 5.76 & \(2.77 \times 10^{-3}\) \\
\hline Benz[ \(a\) ]anthracene & \(2.80 \times 10^{-5}\) & \(5.98 \times 10^{-4}\) & 0.011 & 0.0482 & 1.030 & 5.91 & 0.581 \\
\hline Benzo[b]fluoranthene & & & 0.0015 & 0.00595 & 0.150 & 5.80 & \\
\hline Benzo[j]fluoranthene & & & 0.0025 & 0.0099 & 0.239 & & \\
\hline Benzo[ \(k\) ]fluoranthene & \(5.20 \times 10^{-8}\) & \(3.97 \times 10^{-9}\) & 0.0008 & 0.00317 & 0.242 & 6.00 & 0.016 \\
\hline Benzo[a]pyrene & \(7.00 \times 10^{-7}\) & \(2.38 \times 10^{-5}\) & 0.0038 & 0.0151 & 0.512 & 6.04 & 0.046 \\
\hline Benzo[e]pyrene & \(7.40 \times 10^{-7}\) & \(2.53 \times 10^{-5}\) & 0.004 & 0.0159 & 0.543 & & 0.047 \\
\hline Perylene & \(1.40 \times 10^{-8}\) & \(4.23 \times 10^{-9}\) & 0.0004 & 0.00159 & 0.479 & 6.25 & \(8.83 \times 10^{-3}\) \\
\hline 7,12-DMBA & \(3.84 \times 10^{-8}\) & \(3.45 \times 10^{-7}\) & 0.0500 & 0.195 & 1.757 & 6.00 & \(1.97 \times 10^{-4}\) \\
\hline 9,10-DMBA & \(3.73 \times 10^{-7}\) & \(3.33 \times 10^{-9}\) & 0.0435 & 0.170 & 1.543 & 6.00 & \(2.20 \times 10^{-3}\) \\
\hline 3-MCA & \(1.03 \times 0^{-9}\) & \(3.42 \times 10^{-5}\) & 0.0019 & 0.00708 & 0.235 & 6.42 & 0.145 \\
\hline Benzo[ghi]perylene & & \(2.25 \times 10^{-5}\) & 0.00026 & 0.000941 & 0.252 & 6.50 & \\
\hline Indeno[1,2,3-, c, \(d\) ]pyrene & & & & & & & \\
\hline Dibenz[a,c]anthracene & \(1.30 \times 10^{-9}\) & \(7.84 \times 10^{-8}\) & 0.0016 & 0.00575 & 0.336 & & \(2.26 \times 10^{-4}\) \\
\hline Dibenz \([a, h]\) anthracene & \(3.70 \times 10^{-10}\) & \(9.27 \times 10^{-8}\) & 0.0006 & 0.00216 & 0.540 & 6.75 & \(1.72 \times 10^{-4}\) \\
\hline Dibenz[ \(a, j\) ]anthracene & & & 0.012 & 0.0431 & 2.210 & & \\
\hline Pentacene & \(1.0 \times 10^{-10}\) & & & & & & \\
\hline Coronene & \(2.0 \times 10^{-10}\) & \(2.22 \times 10^{-9}\) & 0.00014 & 0.000466 & 5.179 & 6.75 & \(4.29 \times 10^{-4}\) \\
\hline
\end{tabular}
\begin{tabular}{ll} 
Abbreviations: & \\
3-MCA & 3-Methylcholanthrene \\
7,12-DMBA & 7,12-Dimethylbenz[a]anthracene \\
9,10-DMBA & 9,10-Dimethylbenz[a]anthracene
\end{tabular}

\section*{TABLE 4.2.3 \\ Suggested half-life classes of polynuclear aromatic hydrocarbons (PAHs) in various environment compartments at \(25^{\circ} \mathrm{C}\)}
\begin{tabular}{|c|c|c|c|c|}
\hline Compound & \begin{tabular}{l}
Air \\
class
\end{tabular} & Water class & \begin{tabular}{l}
Soil \\
class
\end{tabular} & Sediment class \\
\hline Indan & 2 & 4 & 6 & 7 \\
\hline Naphthalene & 2 & 4 & 6 & 7 \\
\hline 1-Methyl- & 2 & 4 & 6 & 7 \\
\hline 2,3-Dimethyl- & 2 & 4 & 6 & 7 \\
\hline 1-Ethyl- & 2 & 4 & 6 & 7 \\
\hline 1,4,5-Trimethyl- & 2 & 4 & 6 & 7 \\
\hline Biphenyl & 3 & 4 & 5 & 6 \\
\hline Acenaphthene & 3 & 5 & 7 & 8 \\
\hline Fluorene & 3 & 5 & 7 & 8 \\
\hline Phenanthrene & 3 & 5 & 7 & 8 \\
\hline Anthracene & 3 & 5 & 7 & 8 \\
\hline Pyrene & 4 & 6 & 8 & 9 \\
\hline Fluoranthene & 4 & 6 & 8 & 9 \\
\hline Chrysene & 4 & 6 & 8 & 9 \\
\hline Benz \([a]\) anthracene & 4 & 6 & 8 & 9 \\
\hline Benzo[ \(k\) ]fluoranthene & 4 & 6 & 8 & 9 \\
\hline Benzo[a]pyrene & 4 & 6 & 8 & 9 \\
\hline Perylene & 4 & 6 & 8 & 9 \\
\hline Dibenz \([a, h]\) anthracene & 4 & 6 & 8 & 9 \\
\hline
\end{tabular}
where,
\begin{tabular}{lcc} 
Class & Mean half-life (hours) & Range (hours) \\
1 & 5 & \(<10\) \\
2 & \(17(\sim 1\) day \()\) & \(10-30\) \\
3 & \(55(\sim 2\) days \()\) & \(30-100\) \\
4 & \(170(\sim 1\) week \()\) & \(100-300\) \\
5 & \(550(\sim 3\) weeks \()\) & \(300-1,000\) \\
6 & \(1700(\sim 2\) months \()\) & \(1,000-3,000\) \\
7 & \(5500(\sim 8\) months \()\) & \(3,000-10,000\) \\
8 & \(17000(\sim 2\) years \()\) & \(10,000-30,00\) \\
9 & \(55000(\sim 6\) years \()\) & \(>30,000\)
\end{tabular}


FIGURE 4.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for polynuclear aromatic hydrocarbons.


FIGURE 4.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for polynuclear aromatic hydrocarbons.


FIGURE 4.2.3 Octanol-water partition coefficient versus Le Bas molar volume for polynuclear aromatic hydrocarbons.


FIGURE 4.2.4 Henry's law constant versus Le Bas molar volume for polynuclear aromatic hydrocarbons.


FIGURE 4.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for polynuclear aromatic hydrocarbons.

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[^0]:    *MTC is mass transfer coefficient. Scavenging ratio Q is $2 \times 10^{5}$, dry deposition velocity $\mathrm{U}_{\mathrm{Q}}$ is $10 \mathrm{~m} / \mathrm{h}$ and sediment burial rate $U_{B}$ is $2.0 \times 10^{-7} \mathrm{~m} / \mathrm{h}$

[^1]:    * Assuming $\Delta \mathrm{S}_{\text {fus }}=56 \mathrm{~J} / \mathrm{mol} \mathrm{K}$.

[^2]:    note: $\ln \left(\mathrm{P}_{\mathrm{L}} / \mathrm{P}_{\mathrm{S}}\right)=268.6187-699.31 /(\mathrm{T} / \mathrm{K})-45.6846 \cdot \ln (\mathrm{~T} / \mathrm{K})+0.057217(\mathrm{~T} / \mathrm{K})$; in which $\mathrm{P}_{\mathrm{L}}$ and $\mathrm{P}_{\mathrm{S}}$ are the vapor pressure of supercooled liquid and crystal phase, respectively, at temperature T.

[^3]:    ref. Tsypkina, O.YA. Zh. Prikl. Khim 28, 185 (1955).

