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°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.
Acknowledgments

We would never have completed the volumes for the first and second editions of the handbook and the CD-ROMs without the enormous amount of help and support that we received from our colleagues, publishers, editors, friends, and family. We are long overdue in expressing our appreciation.

We would like first to extend deepest thanks to these individuals: Dr. Warren Stiver, Rebecca Lun, Deborah Tam, Dr. Alice Bobra, Dr. Frank Wania, Ying D. Lei, Dr. Hayley Hung, Dr. Antonio Di Guardo, Qiang Kang, Kitty Ma, Edmund Wong, Jenny Ma, and Dr. Tom Harner. During their past and present affiliations with the Department of Chemical Engineering and Applied Chemistry and/or the Institute of Environment Studies at the University of Toronto, they have provided us with many insightful ideas, constructive reviews, relevant property data, computer know-how, and encouragement, which have resulted in substantial improvements to each consecutive volume and edition through the last fifteen years.

Much credit goes to the team of professionals at CRC Press/Taylor & Francis Group who worked on this second edition. Especially important were Dr. Fiona Macdonald, Publisher, Chemistry; Dr. Janice Shackleton, Input Supervisor; Patricia Roberson, Project Coordinator; Elise Oranges and Jay Margolis, Project Editors; and Marcela Peres, Production Assistant.

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We are grateful to the University of Toronto and Trent University for providing facilities, to the Natural Sciences and Engineering Research Council of Canada and the consortium of chemical companies that support the Canadian Environmental Modelling Centre for funding of the second edition. It is a pleasure to acknowledge the invaluable contributions of Eva Webster and Ness Mackay.
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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.

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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 Introduction

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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 physical-chemical 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 P (Pa) can be viewed as a “solubility in air,” the corresponding concentration C (mol/m³) being P/RT where R is the ideal gas constant (8.314 J/mol.K) and T is absolute temperature (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 $K_{AW}$, the dimensionless ratio of concentration in air (mass/volume) to that in water. The related Henry’s law constant $H$ (Pa.m$^3$/mol) is the ratio of partial pressure in air (Pa) to the concentration in water (mol/m$^3$). 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 $K_{WA}$, the ratio of water-to-air concentrations. This may also be referred to as the Henry’s law constant.

The octanol-water partition coefficient $K_{OW}$ 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 $K_{OC}$, the organic carbon-water partition coefficient, the usual correlation invoked being that of Karickhoff (1981)

$$K_{OC} = 0.41 \, K_{OW}$$

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

$$K_{OC} = 0.35 \, K_{OW}$$

and that the error limits on $K_{OC}$ 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.

$K_{OC}$ 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, $K_{F}$ (sorption partition coefficient to the whole soil on a dry weight basis) and $K_{OM}$ (organic matter-water partition coefficient) are also commonly used to describe the extent of sorption. $K_{OM}$ is often estimated as 0.56 $K_{OC}$, implying that organic matter is 56% carbon.

$K_{OW}$ is also used to estimate equilibrium fish-water bioconcentration factors $K_{FB}$ or BCF using a correlation similar to that of Mackay (1982)

$$K_{FB} = 0.05 \, K_{OW}$$

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., $K_{LW}$ (lipid-water) and $K_{OW}$ are equal. If the rate of metabolism is appreciable, equilibrium will not apply and the effective $K_{FB}$ 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 $pK_a$. 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 $K_{OA}$ 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 $K_{OA}$ than for $K_{OW}$, its use is increasing and when available, data are included in this handbook. $K_{OA}$ 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 $K_{OA}$ 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 $K_{OA}$ to describe partitioning between air and soil.

An attractive feature of $K_{OA}$ is that it can replace the liquid or supercooled liquid vapor pressure in a correlation. $K_{OA}$ 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 $K_{OA}$ 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 $K_{AW}$, $K_{OW}$ and $K_{OA}$ raises the possibility of a consistency test. At first sight it appears that $K_{OA}$ should equal $K_{OW}/K_{AW}$, and indeed this is often approximately correct. The difficulty is that in the case of $K_{AW}$, the water phase is pure water, and for $K_{OA}$ the octanol phase is pure “dry” octanol. For $K_{OW}$ 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 $S$ (mol/m$^3$)

$$K_{AW} = \frac{S_A}{S_W} \text{ or } \log K_{AW} = \log S_A - \log S_W$$

$$K_{OA} = \frac{S_O}{S_A} \text{ or } \log K_{OA} = \log S_O - \log S_A$$

$$K_{OW} = \frac{S_{OW}}{S_{WO}} \text{ or } \log K_{OW} = \log S_{OW} - \log S_{WO}$$

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 $K_{OA}$ is $K_{OW}/K_{AW}$ is essentially that

$$(\log S_{OW} - \log S_O) - (\log S_{WO} - \log S_W) = 0$$

or $S_{OW} S_W/(S_O \cdot S_{WO})$ is 1.0

This is obviously satisfied when $S_{OW}$ equals $S_O$ and $S_{WO}$ equals $S_W$, but this is not necessarily valid, especially when $K_{OW}$ 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 $S_O/S_W$ will be about 0.1 units less than that of log $K_{OW}$. Effectively, the octanol phase “swells” as a result of the presence of water, and the concentration is reduced. In addition, when log $K_{OW}$ exceeds 4.0 there is an apparent effect on the activity coefficients which causes log $(S_O/S_W)$ to increase. This increase can amount to about one log unit when log $K_{OW}$ is about 8. A relatively simple correlation based on the analysis by Beyer et al. (2002) (but differing from their correlation) is that

$$\log K_{OA} = \log \left(\frac{K_{OW}}{K_{AW}}\right) - 0.10 + [0.30 \log K_{OW} - 1.20]$$

when log $K_{OW}$ is 4 or less the term in square brackets is ignored

when log $K_{OW}$ is 4 or greater that term is included

### 1.2.3 Temperature Dependence

All partitioning properties change with temperature. The partition coefficients, vapor pressure, $K_{AW}$ and $K_{OA}$, 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 $K_p$,

$$R \cdot \ln K_p = A \rho - B/T$$

which can be rewritten as

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

where $A$, $B$ 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),

\[
R \ln K_{p}(T) = A + B/T + C \ln T + DT^2 + ET^3 + ...... 
\]

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):

\[
d(ln x)/dT = – \Delta_{sol}H/R 
\]

where \(x\) is the mole fraction solubility, \(T\) is the temperature in K, \(R\) is the ideal gas constant, and \(\Delta_{sol}H\) 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,

\[
ln x = – \Delta_{sol}H/RT + C 
\]

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,

\[
d(ln P^S)/dT = \Delta_{vap}H/RT^2 
\]

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

\[
ln P^S = – \Delta_{vap}H/RT + C 
\]

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, Boublík 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 °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., $p/\alpha$ or $p/\alpha$ 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

$$\ln \left( \frac{k_H}{Pa} \right) = \ln \left[ \left( \frac{P^g}{Pa} \right) x \right]$$

or,

$$\ln \left( \frac{H}{Pa \cdot m^3 \cdot mol^{-1}} \right) = \ln \left[ \left( \frac{P^g}{Pa} \right) \left( \frac{CS_w}{mol \cdot m^{-3}} \right) \right]$$

where $CS_w$ 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, $K_a$, expressed as its negative logarithm, $pK_a$, 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 $pK_a$ 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,

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

The fraction ionic $x_I$ is $I/(1 + I)$. The fraction non-ionic $x_N$ is $1/(1 + I)$. For compounds such as pentachlorophenol in which pH generally exceeds $pK_a$, $I$ and $x_N$ 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), biocentration and uptake kinetics to goldfish (Steely 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 $x_I$ and the fraction non-ionic $x_N$ for the chemical at both the pH and temperature of experimental data determination ($I_{exp}, x_{ID}, x_{ND}$) and at the pH and temperature of the desired environmental simulation ($I_{esp}, x_{IEP}, x_{NEP}$). 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 $H^+$. This approach must be regarded as merely a first correction for the dissociation effect. An accurate evaluation should preferably be based on experimental
The solubility and $K_{ow}$ of the non-ionic forms can be estimated as

$$C_N = C_T \gamma_{ND}; \quad K_{OW,N} = K_{OW,T}/\gamma_{ND}$$

Vapor pressure $P^S$ is not affected, but the apparent Henry’s law constant $H_N$ must also be adjusted to $H_N/\gamma_N$, being $P^S/C_N^S$ or $P^S/(C_T^S \gamma_N)$.

$C_N$ and $K_{OW,N}$ can be applied to environmental conditions with a temperature adjustment if necessary. Values of $I_E \gamma_N$ and $\gamma_{ND}$ can be deduced from the environmental pH and the solubility and $K_{ow}$ 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 $K_{AW}$ 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 $K_{AW}$ directly. If the chemical’s activity coefficient $\gamma$ in water is known, then $H$ can be estimated as $\gamma_{w}P_{w}^S$, where $\gamma_{w}$ is the molar volume of water and $P_{w}^S$ is the liquid vapor pressure. Since $H$ can be regarded as $P_{w}^S/C_{w}^S$, where $C_{w}^S$ is the solubility, it is apparent that $(1/\gamma_{w}P_{w}^S)$ 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 mol/m$^3$ since the molar volume of water $v_w$ is $18 \times 10^{-6}$ m$^3$/mol or 18 cm$^3$/mol. Chemicals with $\gamma$ less than about 20 are usually miscible in water. If the liquid vapor pressure in this case is 1000 Pa, $H$ will be 1000/11100 or 0.090 Pa·m$^3$/mol and $K_{AW}$ will be $HRT$ or $3.6 \times 10^{-5}$ at 25°C. Alternatively, if $H$ or $K_{AW}$ is known, $C_{w}^S$ 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., $C_{w}^S$, $P_{w}^S/H$ or $P_{w}^S$ or $K_{AW}$-$RT$). 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 Jaouï 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°C, which exceeds atmospheric pressure of 101325 Pa, the boiling point being –42°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°C. Benzene, for example, has a critical temperature of 562 K, a boiling point of 80°C and a vapor pressure of 12700 Pa at 25°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 $K_{AW}$ 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°C and at 25°C the solid has a solubility in water of 33 g/m³ and a vapor pressure of 10.9 Pa. If naphthalene was a liquid at 25°C it is estimated that its solubility would be 115 g/m³ 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°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 liquid-like state on or in the aerosol particle. It does not exist in crystalline form.

When calculating partition coefficients such as $K_{AW}$, $K_{OW}$ or $K_{OA}$ 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 $T$ (K) from the expression

$$\ln F = -\Delta S (T_M - T)/RT$$

where $\Delta S$ is the entropy of fusion, $T_M$ is the melting point, and $R$ is the gas constant. $\Delta S$ is related to the measurable enthalpy of fusion $\Delta H$ at the melting point as $\Delta H/T_M$. The reader should use experimental data for $\Delta H$, $\Delta S$ and melting point whenever possible. The most reliable method is to measure $\Delta H$ calorimetrically, calculate $\Delta S$ and use this value to estimate $F$. Only in the absence of $\Delta H$ data should a QSPR be used or Walden’s Rule applied that $\Delta S$ is approximately 56.5 J/mol K. This assumption leads to the equations

$$F = \exp(-6.79(T_M/T - 1))$$
$$\log F = -0.01(T_M - 298)$$
F is thus 1.0 at the melting point, with lower values at lower temperatures. It is not applied at temperatures exceeding \( T_M \).

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.

<table>
<thead>
<tr>
<th>class</th>
<th>mean half-life (hours)</th>
<th>range (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5 &lt; 10</td>
<td>10–30</td>
</tr>
<tr>
<td>2</td>
<td>17 (∼ 1 day)</td>
<td>30–100</td>
</tr>
<tr>
<td>3</td>
<td>55 (∼ 2 days)</td>
<td>100–300</td>
</tr>
<tr>
<td>4</td>
<td>170 (∼ 1 week)</td>
<td>300–1,000</td>
</tr>
<tr>
<td>5</td>
<td>550 (∼ 3 weeks)</td>
<td>1,000–3,000</td>
</tr>
<tr>
<td>6</td>
<td>1700 (∼ 2 months)</td>
<td>3,000–10,000</td>
</tr>
<tr>
<td>7</td>
<td>5500 (∼ 8 months)</td>
<td>10,000–30,000</td>
</tr>
<tr>
<td>8</td>
<td>17000 (∼ 2 years)</td>
<td>30,000–100,000</td>
</tr>
<tr>
<td>9</td>
<td>55000 (∼ 6 years)</td>
<td>&gt; 100,000</td>
</tr>
<tr>
<td>10</td>
<td>&gt; 11 years</td>
<td></td>
</tr>
</tbody>
</table>

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 h\(^{-1}\)) and simultaneous photolysis with a rate constant of 0.0011 h\(^{-1}\) (half-life 630 hours). The overall rate constant is thus 0.0025 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 cm\(^3\)). The product of the assumed hydroxyl radical concentration and the second-order 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 (OH), ozone (O\(_3\)) and nitrate radicals (NO\(_3\)) 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.
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 oxygen-containing organics. In addition, photooxidation reactions with O₃ and NOₓ radicals can result in transformation of these compounds. The night-time reaction with NOₓ 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 peroxyl 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 this 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 $pK_a$

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 g/100 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 to 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, Chiu 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 $K_a$ or its commonly reported negative logarithmic form $pK_a$ 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 mg/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, e.g., comparative ebulliometry (Ambrose 1981);
   c. Effusion methods, torsion and weight-loss (Balson 1947, Bradley and Cleasby 1953, Hamaker and Kerlinger 1969, De Kruif 1980);
   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);

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 \( K_{OW} \)

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 \( C_O/C_W \). This is actually the ratio of solute concentration in octanol saturated with water to that in water saturated with octanol.

As with solubility, \( K_{OW} \) 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 \( K_{OW} \) from molecular structure; thus, there has been a tendency to calculate \( K_{OW} \) 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 \( K_{OW} \) 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, \( K_{OW} \) is low and can be less than 1.0, resulting in negative values of \( \log K_{OW} \). 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 Andre (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 (Vejriosta et al. 1982, Jönnsson 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 \( \gamma^* \) (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 \( K_{OA} \)**

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, \( K_{OW} \), \( K_{AW} \), \( K_{OA} \), 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 cm\(^3\)/mol (Reid et al. 1987). From the above rules, the Le Bas molar volume for chlorobenzene (\( C_6H_5Cl \)) is:

\[
V = 6 \times 14.8 + 5 \times 3.7 + 24.6 - 15 = 117 \text{ cm}^3/\text{mol}
\]

Accordingly, plots are presented at the end of each chapter for solubility, vapor pressure, \( K_{OW} \) and Henry’s law constant versus Le Bas molar volume.
Introduction

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 J/mol·K or 13.5 cal/mol·K (e.u.)

\[
F = \frac{C_S}{C_L} = \frac{P_S}{P_L} = \exp\{6.79(1 - T_M/T)\}
\]

where \( C_S \) is solubility, \( P_S \) is vapor pressure, subscripts S and L refer to solid and liquid phases, \( T_M \) 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°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 physical-chemical 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).

---

**TABLE 1.3.1**
Le Bas molar volume

<table>
<thead>
<tr>
<th>increment, cm³/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
</tr>
<tr>
<td>Hydrogen</td>
</tr>
<tr>
<td>Oxygen</td>
</tr>
<tr>
<td>- In methyl esters and ethers</td>
</tr>
<tr>
<td>- In ethyl esters and ethers</td>
</tr>
<tr>
<td>- Join to S, P, or N</td>
</tr>
<tr>
<td>Nitrogen</td>
</tr>
<tr>
<td>- Doubly bonded</td>
</tr>
<tr>
<td>- In primary amines</td>
</tr>
<tr>
<td>- In secondary amines</td>
</tr>
<tr>
<td>Bromine</td>
</tr>
<tr>
<td>Chlorine</td>
</tr>
<tr>
<td>Fluorine</td>
</tr>
<tr>
<td>Iodine</td>
</tr>
<tr>
<td>Sulfur</td>
</tr>
<tr>
<td>Rings</td>
</tr>
<tr>
<td>- Three-membered</td>
</tr>
<tr>
<td>- Four-membered</td>
</tr>
<tr>
<td>- Five-membered</td>
</tr>
<tr>
<td>- Six-membered</td>
</tr>
<tr>
<td>- Naphthalene</td>
</tr>
<tr>
<td>- Anthracene</td>
</tr>
</tbody>
</table>
Examples are Burkhard (1984) and Burkhard et al. (1985a), who calculated solubility, vapor pressure, Henry’s law constant, $K_{ow}$ and $K_{oc}$ for all PCB congeners. Hawker and Connell (1988) also calculated $\log K_{ow}$; 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 $K_{ow}$ 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, $K_{ow}$ 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, $\log K_{ow}$ and toxicity of organic chemicals. Warne et al. (1990) correlated solubility and $K_{ow}$ 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](http://www.syrres.com).

For correlation of solubility, the correct thermodynamic quantities for correlation are the activity coefficient $\gamma$, or the excess Gibbs free energy $\Delta G$, 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 cm$^3$/mol
   - Liquid molar volume - from density (McAuliffe 1966, Lande and Banerjee 1981, Chiou et al. 1982, Abernethy et al. 1988, Wang et al. 1992);
   - Molar volume by additive group contribution method, e.g., Le Bas method, Schroeder method (Reid et al. 1987, Miller et al. 1985);
   - Intrinsic molar volume, $V_I$, cm$^3$/mol - from van der Waals radius with solvatochromic parameters $\alpha$ and $\beta$ (Leahy 1986, Kamlet et al. 1987, 1988);
   - Characteristic molecular volume, m$^3$/mol (McGowan and Mellors 1986);
4. Molecular volume - Å$^3$/molecule (cubic Angstrom per molecule)
   - van der Waals volume (Bondi 1964);
   - Total molecular volume (TMV) (Pearlman et al. 1984, Pearlman 1986);
6. Molecular connectivity indices (MCI) or $\chi$ (Kier and Hall 1976, Andre 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 Ballschmitter 1988);
11. Adsorbability index (AI) (Okouchi et al. 1992);

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.


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 $K_{OW}$ is widely used as a descriptor of hydrophobicity. Variation in $K_{OW}$ 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 $K_{OW}$. Most widely used is the Hansch-Leo compilation of data (Leo et al. 1971, Hansch and Leo 1979) and related predictive methods. Examples of $K_{OW}$ 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);
   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 - $K_{OW}$ 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).


7. Combination of HPLC retention data and molecular connectivity indices (Finizio et al. 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 Clausius-Clapeyron, 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 $T_B$ and heat of vaporization $\Delta H_v$ (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 $\Delta G_v$ (Burkhard et al. 1985a);
8. TSA and $\Delta G_v$ (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 $T_m$ and GC retention index (Bidleman 1984, Burkhard et al. 1985a);

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, $K_{ow}$ 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);

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

**Bioconcentration Factors:**

3. Correlation with $K_{oc}$ (Kenaga 1980, Kenaga and Goring 1980, Briggs 1981);
4. Calculation with HPLC retention data (Swann et al. 1983);

**Sorption Coefficients:**

1. Correlation with $K_{ow}$ (Karickhoff et al. 1979, Schwarzenbach and Westall 1981, Mackay 1982, Oliver 1984);
2. Correlation with solubility (Karickhoff et al. 1979);
4. Estimation from molecular connectivity index/fragment contribution method (Meylan et al. 1992, Lohninger 1994);

**Octanol-Air Partition coefficient.**

The molecular descriptors used for $K_{ow}$ solubility in water and vapor pressure can potentially be applied to $K_{oa}$.

### 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 km² or 10¹¹ m², 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 km² is used, with a water depth of 20 m. The water volume is thus 2 × 10¹¹ m³. 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 × 10⁹ m³. 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 10⁸ m³.

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 × 10⁻⁶, i.e., it is about 5 to 10 mg/L. The volume is thus 10⁶ m³. 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 × 10⁵ m³. 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 × 10⁻¹¹, i.e., approximately 30 µg/m³. 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 kg or 100 tonnes. If dispersed entirely in the air, this amount yields a concentration of 1 µg/m³ which is not unusual for ubiquitous contaminants such as hydrocarbons. If dispersed entirely in the water, the concentration is a higher 500 µg/L which again is reasonable for a well-used chemical of commerce. 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

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Air</th>
<th>Water</th>
<th>Soil</th>
<th>Sediment</th>
<th>Suspended sediment</th>
<th>Fish</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume, V (m³)</td>
<td>10¹⁴</td>
<td>2 × 10¹¹</td>
<td>9 × 10⁹</td>
<td>10⁸</td>
<td>10⁶</td>
<td>2 × 10⁸</td>
</tr>
<tr>
<td>Depth, h (m)</td>
<td>1000</td>
<td>20</td>
<td>0.1</td>
<td>0.01</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Area, A (m²)</td>
<td>100 × 10⁹</td>
<td>10 × 10⁹</td>
<td>90 × 10⁹</td>
<td>10 × 10⁹</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Fraction OC</td>
<td>—</td>
<td>—</td>
<td>0.02</td>
<td>0.04</td>
<td>0.2</td>
<td>—</td>
</tr>
<tr>
<td>Density, ρ (kg/m³)</td>
<td>1.2</td>
<td>1000</td>
<td>2400</td>
<td>2400</td>
<td>1500</td>
<td>1000</td>
</tr>
<tr>
<td>Adv. Residence</td>
<td>100</td>
<td>1000</td>
<td>—</td>
<td>50,000</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Adv. flow, G (m³/h)</td>
<td>10¹²</td>
<td>2 × 10⁸</td>
<td>—</td>
<td>2000</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>
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 (Pa) common to all media is deduced as

\[ f = M/\Sigma V Z_i \]

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

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>Total volume</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Air phase</td>
<td></td>
</tr>
<tr>
<td>Aerosol phase</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>Total volume</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Water phase</td>
<td></td>
</tr>
<tr>
<td>Suspended sediment phase</td>
<td></td>
</tr>
<tr>
<td>Fish phase</td>
<td></td>
</tr>
<tr>
<td>Soil</td>
<td>Total volume</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Air phase</td>
<td></td>
</tr>
<tr>
<td>Water phase</td>
<td></td>
</tr>
<tr>
<td>Solid phase</td>
<td></td>
</tr>
<tr>
<td>Sediment</td>
<td>Total volume</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Water phase</td>
<td></td>
</tr>
<tr>
<td>Solid phase</td>
<td></td>
</tr>
</tbody>
</table>

\[ f = \frac{M}{\Sigma V Z_i} \]

Note for solids $P_S^L = P_G^L / \exp\{6.79(1 - T_m/T)\}$, where $T_m$ is melting point (K) of the solute and T is 298 K. An experimental entropy of fusion should be used if available.

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

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Z values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>$Z_a = 1/RT$</td>
</tr>
<tr>
<td>Water</td>
<td>$Z_w = 1/H = C^S/P_S^S$</td>
</tr>
<tr>
<td>Soil</td>
<td>$Z_s = Z_w^2 \rho_s \phi_s K_{OC}/1000$</td>
</tr>
<tr>
<td>Sediment</td>
<td>$Z_s = Z_w^2 \rho_s \phi_s K_{OC}/1000$</td>
</tr>
<tr>
<td>Suspended Sediment</td>
<td>$Z_{ss} = Z_w^2 \rho_{ss} \phi_{ss} K_{OC}/1000$</td>
</tr>
<tr>
<td>Fish</td>
<td>$Z_f = Z_w^2 \rho \phi L K_{OW}/1000$</td>
</tr>
<tr>
<td>Aerosol</td>
<td>$Z_a = Z_w^2 \rho \phi_L K_{OA}$</td>
</tr>
</tbody>
</table>

where

- $R$ = gas constant (8.314 J/mol·K)
- $T$ = absolute temperature (K)
- $C^S$ = solubility in water (mol/m$^3$)
- $P_S^S$ = vapor pressure (Pa)
- $H$ = Henry’s law constant (Pa·m$^3$/mol)
- $P_G^L$ = liquid vapor pressure (Pa)
- $K_{OA}$ = octanol-air partition coefficient
- $K_{OW}$ = octanol-water partition coefficient
- $\rho_i$ = density of phase i (kg/m$^3$)
- $\phi_i$ = mass fraction organic-carbon in phase i (g/g)
- $L$ = lipid content of fish

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where M is the total amount of chemical (mol), \( V_i \) is the medium volume (m\(^3\)) and \( Z_i \) 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 \( C \) (mol/m\(^3\)) can then be deduced as \( Z_f \) mol/m\(^3\) or as \( WZ_f \) g/m\(^3\) or \( 1000 WZ_f/\rho \) µg/g, where \( \rho \) is the phase density (kg/m\(^3\)) and W is the molecular mass (g/mol). The amount \( m_i \) in each medium is \( C_iV_i \) 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 pH). The total \( Z \) value in water is then separated into its ionic and non-ionic contributions, i.e., fractions of \( I/(I + 1) \) and \( l/(l + I) \). 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 g/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 \( K_{ow} \) and Henry’s law constant and the air-water partition coefficient, and decreasing the soil-water partition coefficient.

**Note:** At pH of 5.1, \( K_{ow} \) is 112200 and is the ratio of concentration in octanol to total concentration in water comprising fractions \( I/(I + 1) \) or \( l/(l + 2.29) \) or 0.157 of neutral and 0.843 of ionic species. \( K_{ow} \) is thus 112200/0.304 or 369000 for the neutral species and zero for the ionic species. For the neutral species \( K_{oc} \) is assumed to be 0.41 \( K_{ow} \) or 151300, thus \( K_p \) is 151300 \times 0.02 L/kg, i.e., 3027 for a soil of 2% organic carbon. \( K_{ow} \) is thus 3027 \times 2.4 where 2.4 is the solid density (kg/L) or 7265. \( Z_s \) for the neutral species is thus 7265 \times Z_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. \( K_{ow} \) thus decreases to 27970/704 or 39.72.

**TABLE 1.5.4**

Bulk phase \( Z \) values, \( Z_{Bi} \) deduced as \( \sum_v Z_i \), 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

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Bulk ( Z ) values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>( Z_{B1} = Z_1 + 2 \times 10^{-11} Z_7 ) (approximately 30 µg/m(^3) aerosols)</td>
</tr>
<tr>
<td>Water</td>
<td>( Z_{B2} = Z_2 + 5 \times 10^{-6} Z_5 + 1 \times 10^{-6} Z_6 ) (5 ppm solids, 1 ppm fish by volume)</td>
</tr>
<tr>
<td>Soil</td>
<td>( Z_{B3} = 0.2 Z_1 + 0.3 Z_2 + 0.5 Z_3 ) (20% air, 30% water, 50% solids)</td>
</tr>
<tr>
<td>Sediment</td>
<td>( Z_{B4} = 0.8 Z_2 + 0.2 Z_4 ) (80% water, 20% solids)</td>
</tr>
</tbody>
</table>

**TABLE 1.5.5**

Calculated \( Z \) values at different experimental and environmental pHs of pentachlorophenol. \( Z \) values at 25°C, \( \log K_{ow} \) is 5.05, \( pK_a \) 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 kg/L

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Neutral</th>
<th>Ionic</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>At data pH of 5.1 (( l = 2.29 ))</td>
<td>( 4.03 \times 10^{-4} )</td>
<td>0</td>
<td>( 4.03 \times 10^{-4} )</td>
</tr>
<tr>
<td>Air</td>
<td>3.85</td>
<td>8.82</td>
<td>12.67</td>
</tr>
<tr>
<td>Water</td>
<td>27970</td>
<td>0</td>
<td>27970</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Neutral</th>
<th>Ionic</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>At environ. pH of 7 (( l = 182 ))</td>
<td>4.03 \times 10^{-4}</td>
<td>0</td>
<td>4.03 \times 10^{-4}</td>
</tr>
<tr>
<td>Air</td>
<td>3.85</td>
<td>700.4</td>
<td>704.2</td>
</tr>
<tr>
<td>Water</td>
<td>27970</td>
<td>0</td>
<td>27970</td>
</tr>
</tbody>
</table>
This is further demonstrated in Table 1.5.6 which shows the effects of environmental pH on the partitioning behavior of pentachlorophenol (PCP), 2,4-dichlorophenol (2,4-DCP), 2,4,6-trichlorophenol (2,4,6-TCP) and p-cresol at 25°C. $K_{aw}$ is the air-water partition coefficient and $K_{sw}$ is the soil-water partition coefficient.

**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°C. $K_{aw}$ is the air-water partition coefficient and $K_{sw}$ is the soil-water partition coefficient.

<table>
<thead>
<tr>
<th>At pH</th>
<th>Neutral $Z_w$</th>
<th>Ionic $Z_w$</th>
<th>Total $Z_w$</th>
<th>Fraction $x_N$</th>
<th>$S_t$ g/m³</th>
<th>$H_t$ Pa·m³/mol</th>
<th>$K_{aw}$</th>
<th>$K_{sw}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.849</td>
<td>0.7004</td>
<td>4.549</td>
<td>0.846</td>
<td>16.55</td>
<td>0.224</td>
<td>8.9 × 10⁻⁵</td>
<td>6147</td>
</tr>
<tr>
<td>6</td>
<td>3.849</td>
<td>70.04</td>
<td>73.89</td>
<td>0.052</td>
<td>268.8</td>
<td>0.0135</td>
<td>5.46 × 10⁻⁶</td>
<td>378.5</td>
</tr>
<tr>
<td>7</td>
<td>3.849</td>
<td>700.4</td>
<td>704.2</td>
<td>0.0055</td>
<td>2562</td>
<td>0.00142</td>
<td>5.73 × 10⁻⁷</td>
<td>39.7</td>
</tr>
<tr>
<td>4</td>
<td>1.7677</td>
<td>0.0140</td>
<td>1.7817</td>
<td>0.992</td>
<td>434</td>
<td>0.5612</td>
<td>2.26 × 10⁻⁴</td>
<td>105.2</td>
</tr>
<tr>
<td>6</td>
<td>1.7677</td>
<td>1.4041</td>
<td>3.1718</td>
<td>0.557</td>
<td>772</td>
<td>0.315</td>
<td>1.272 × 10⁻⁴</td>
<td>59.09</td>
</tr>
<tr>
<td>7</td>
<td>1.7677</td>
<td>14.041</td>
<td>15.8088</td>
<td>0.118</td>
<td>3644</td>
<td>0.172</td>
<td>6.945 × 10⁻⁵</td>
<td>11.86</td>
</tr>
<tr>
<td>4</td>
<td>3.063</td>
<td>0.000386</td>
<td>3.063</td>
<td>1.0</td>
<td>6000</td>
<td>0.326</td>
<td>0.000132</td>
<td>31.24</td>
</tr>
<tr>
<td>6</td>
<td>3.063</td>
<td>0.0386</td>
<td>3.101</td>
<td>0.988</td>
<td>6073</td>
<td>0.322</td>
<td>0.000130</td>
<td>30.85</td>
</tr>
<tr>
<td>7</td>
<td>3.063</td>
<td>0.386</td>
<td>3.448</td>
<td>0.888</td>
<td>6760</td>
<td>0.290</td>
<td>0.000117</td>
<td>27.75</td>
</tr>
<tr>
<td>4</td>
<td>11.97</td>
<td>0</td>
<td>11.948</td>
<td>1.0</td>
<td>22000</td>
<td>0.0836</td>
<td>3.37 × 10⁻⁵</td>
<td>1.968</td>
</tr>
<tr>
<td>7</td>
<td>11.97</td>
<td>0.0066</td>
<td>11.975</td>
<td>1.0</td>
<td>22000</td>
<td>0.0836</td>
<td>3.35 × 10⁻⁵</td>
<td>1.968</td>
</tr>
</tbody>
</table>

This is further demonstrated in Table 1.5.6 which shows the effects of environmental pH on the partitioning behavior of 2,4-dichlorophenol (pKₐ = 7.90, solubility of 6000 g/m³ at pH of 5.1 and log $K_{ow}$ = 3.20), 2,4,6-trichlorophenol (pKₐ = 6.10, solubility of 430 g/m³ at pH of 5.1 and log $K_{ow}$ = 3.69), pentachlorophenol (pKₐ = 4.74, solubility of 14.0 g/m³ at pH of 5.1 and log $K_{ow}$ = 5.05) and p-cresol (pKₐ = 10.26, a solubility of 22000 g/m³ and log $K_{ow}$ = 2.0) in the multimedia environment at 25°C. For environmental pH from 4 to 7, there is no significant effect for p-cresol (or for chemicals for which pKₐ >> pH), very little effect for 2,4-dichlorophenol (and chemicals with pKₐ ranging between 7–10). There is some effect on 2,4,6-trichlorophenol (and chemicals with pKₐ 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 pKₐ is defined as (14 - pK_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 $k_i$ h⁻¹ are used to calculate reaction D values for each medium $D_{ri}$ as $V_iZ_i k_i$. The rate of reactive loss is then $D_{rif}$ mol/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 $V_it$ m³/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 $D_{ai}$ is $G_itZ_i$, and the rates are $D_{aif}$ mol/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 $E$ mol/h can be equated to the sum of the output rates, from which the common fugacity can be calculated as follows:

$$E = f \Sigma D_{Ai} + f \Sigma D_{Ri}$$

thus,

$$f = E / (\Sigma D_{Ai} + \Sigma D_{Ri})$$

The common assumed emission rate is 1000 kg/h or 1 tonne/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 $m_i$ and $\Sigma m_i$ 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

$$t_O = M / E$$

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

$$t_R = M / \Sigma D_{Ri} f \quad t_A = M / \Sigma D_{Ai} f$$

Obviously,

$$1/t_O = 1/t_R + 1/t_A$$

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 (m/h or m/year), are designated as $U_i$ m/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 $(D_{12})$

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 \((k_w)\) and air-side \((k_a)\) mass transfer coefficients \((\text{m/h})\) being defined. Values of 0.05 m/h for \(k_w\) and 5 m/h for \(k_a\) are used. The absorption \(D\) value is then

\[
D_{vw} = 1\left[\frac{1}{k_a A_w Z_1} + \frac{1}{k_w A_w Z_2}\right]
\]

where \(A_w\) is the air-water area \((\text{m}^2)\) and \(Z_1\) and \(Z_2\) are the pure air and water \(Z\) values. The velocities \(k_a\) and \(k_w\) are designated as \(U_1\) and \(U_2\).

For rain dissolution, a rainfall rate of 0.876 m/year is used, i.e., \(U_R\) or \(U_3\) is \(10^{-4}\) m/h. The \(D\) value for rain dissolution \(D_{rw}\) is then

\[
D_{rw} = U_R A_w Z_2 = U_3 A_w Z_2
\]

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) \(v_Q\) of \(2 \times 10^{-11}\), this corresponds to the removal of \(Q v_Q\) or \(4 \times 10^{-6}\) volumes of aerosol per volume of rain. The total rate of particle removal by wet deposition is then \(Q v_Q U_R A_w\) m³/h, thus the wet “transport velocity” \(Q v_Q U_R\) is \(4 \times 10^{-10}\) m/h.

For dry deposition, a typical deposition velocity \(U_Q\) of 10 m/h is selected yielding a rate of particle removal of \(U_Q v_Q A_w\) or \(2 \times 10^{-10} A_w\) m³/h corresponding to a transport velocity of \(2 \times 10^{-10}\) m/h. Thus,

\[
U_4 = Q v_Q U_R + U_Q v_Q = v_Q (Q U_R + U_Q)
\]

The total particle transport velocity \(U_4\) for wet and dry deposition is thus \(6 \times 10^{-10}\) m/h \((67\% \text{ wet and } 33\% \text{ dry})\) and the total \(D\) value \(D_{qw}\) is

\[
D_{qw} = U_4 A_w Z_7
\]

where \(Z_7\) is the aerosol \(Z\) value.

The overall \(D\) value is given by

\[
D_{12} = D_{vw} + D_{rw} + D_{qw}
\]

2. Water to Air (\(D_{21}\))
Evaporation is treated as the reverse of absorption; thus \(D_{21}\) is simply \(D_{vw}\) 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 \(D_{rs}\) and wet and dry deposition \(D_{qs}\) being treated identically except that the area term is now the air-soil area \(A_s\).

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 \(k_s\) or \(U_7\) of 5 m/h, equal to that of the air-water mass transfer coefficient \(k_a\) used in \(D_{12}\).

For diffusion in the soil air-pores, a molecular diffusivity of 0.02 m²/h is reduced to an effective diffusivity using a Millington-Quirk type of relationship by a factor of about 20 to \(10^{-3}\) m²/h. Combining this with a path length of 0.05 m gives an effective air-to-soil mass transfer coefficient \(k_{sa}\) of 0.02 m/h, which is designated as \(U_s\).

Similarly, for diffusion in water a molecular diffusivity of \(2 \times 10^{-6}\) m²/h is reduced by a factor of 20 to an effective diffusivity of \(10^{-7}\) m²/h, which is combined with a path length of 0.05 m to give an effective soil-to-water mass transfer coefficient of \(k_{sw}\) \(2 \times 10^{-6}\) m/h.

It is probable that capillary flow of water contributes to transport in the soil. For example, a rate of 7 cm/year would yield an equivalent water velocity of \(8 \times 10^{-6}\) m/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 \(10 \times 10^{-6}\) m/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

\[
D_{vs} = 1\left[1/D_s + 1/(D_{sw} + D_{sa})\right]
\]
where

\[
D_S = U_8 A_S Z_1 \quad (U_7 = 5 \text{ m/h})
\]

\[
D_{SW} = U_6 A_{SW} Z_2 \quad (U_6 = 10 \times 10^{-6} \text{ m/h})
\]

\[
D_{SA} = U_9 A_S Z_1 \quad (U_5 = 0.02 \text{ m/h})
\]

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

\[
D_{13} = D_{VS} + D_{QS} + D_{RS}
\]

**4. Soil to Air (D_{31})**

Evaporation is treated as the reverse of absorption, thus the D value is simply \(D_{VS}\).

**5. Water to Sediment (D_{24})**

Two processes are treated, diffusion and deposition.

Diffusion is characterized by a mass transfer coefficient \(U_8\) of \(10^{-4}\) m/h, which can be regarded as a molecular diffusivity of \(2 \times 10^{-6}\) m²/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 \(U_8 A_W Z_2\).

Deposition is assumed to occur at a rate of 5000 m³/h, which corresponds to the addition of a depth of solids of 0.438 cm/year; thus 43.8% of the solids resident in the accessible bottom sediment is added each year. This rate is about 12 cm²/m²-day, which is high compared to values observed in large lakes. The velocity \(U_9\), corresponding to the addition of 5000 m³/h over the area of \(10^{10}\) m², is thus \(5 \times 10^{-7}\) m/h.

It is assumed that of this 5000 m³/h deposited, 2000 m³/h or 40% is buried (yielding the advective flow rate in Table 1.5.1), 2000 m³/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:

- deposition \(U_9\) \(5.0 \times 10^{-7}\) m/h or 0.438 cm/y
- resuspension \(U_{10}\) \(2.0 \times 10^{-7}\) m/h or 0.175 cm/y
- burial \(U_9\) \(2.0 \times 10^{-7}\) m/h or 0.175 cm/y

\((\text{included as an advective residence time of } 50,000 \text{ h})\)

The water-to-sediment D value is thus

\[
D_{24} = U_8 A_W Z_2 + U_9 A_W Z_4
\]

where \(Z_4\) is the Z value of the particles in the water column.

**6. Sediment to Water (D_{42})**

This is treated similarly to \(D_{24}\) giving:

\[
D_{42} = U_8 A_W Z_2 + U_{10} A_W Z_4
\]

where \(U_{10}\) is the sediment resuspension velocity of \(2.0 \times 10^{-7}\) m/h and \(Z_4\) is the Z value of the sediment solids.
7. Sediment Advection or Burial ($D_{44}$)

This $D$ value is $U_B A_W Z_4$, where $U_B$, the sediment burial rate, is $2.0 \times 10^{-7}$ m/h. It can be viewed as $G_B Z_{44}$, where $G_B$ is the total burial rate specified as $V_S/t_B$ where $t_B$ (residence time) is 50,000 h, and $V_S$ (the sediment volume) is the product of sediment depth (0.01 cm) and area $A_W$. $Z_{44}$ are the $Z$ values of the sediment solids and of the bulk sediment, respectively. Since there are 20% solids, $Z_{44}$ is about 0.2 $Z_4$. 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 ($D_{32}$)

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

$$D = 0.5 U_3 A_W Z_2 = U_3 A_W Z_2$$

thus the transport velocity term $U_{31}$ is $0.5U_3$ or $5 \times 10^{-5}$ m/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 $U_{12}$ is $200 \times 10^{-6} U_{11}$, i.e., $10^{-8}$ m/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 1/10th 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 kg/h) are introduced individually into air, soil and water. Direct discharges to sediment are unlikely and are not

<table>
<thead>
<tr>
<th>Table 1.5.7</th>
<th>Intermedia transport parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>U</strong></td>
<td>m/h</td>
</tr>
<tr>
<td>1</td>
<td>Air side, air-water MTC* $k_A$</td>
</tr>
<tr>
<td>2</td>
<td>Water side, air-water MTC, $k_W$</td>
</tr>
<tr>
<td>3</td>
<td>Rain rate, $U_R$</td>
</tr>
<tr>
<td>4</td>
<td>Aerosol deposition</td>
</tr>
<tr>
<td>5</td>
<td>Soil-air phase diffusion MTC, $k_{SA}$</td>
</tr>
<tr>
<td>6</td>
<td>Soil-water phase diffusion MTC, $k_{SW}$</td>
</tr>
<tr>
<td>7</td>
<td>Soil-air boundary layer MTC, $k_S$</td>
</tr>
<tr>
<td>8</td>
<td>Sediment-water MTC</td>
</tr>
<tr>
<td>9</td>
<td>Sediment deposition</td>
</tr>
<tr>
<td>10</td>
<td>Sediment resuspension</td>
</tr>
<tr>
<td>11</td>
<td>Soil-water run-off</td>
</tr>
<tr>
<td>12</td>
<td>Soil-solids run-off</td>
</tr>
</tbody>
</table>

* MTC is mass transfer coefficient. Scavenging ratio $Q$ is $2 \times 10^5$, dry deposition velocity $U_Q$ is $10$ m/h and sediment burial rate $U_B$ is $2.0 \times 10^{-7}$ m/h
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.

### TABLE 1.5.8

**Intermedia transport D value equations**

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Mass balance equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air-Water</td>
<td>( D_{12} = D_{vw} + D_{rw} + D_{qw} )</td>
</tr>
<tr>
<td></td>
<td>( D_{vw} = A_w(1/U_1 Z_1 + 1/U_2 Z_2) )</td>
</tr>
<tr>
<td></td>
<td>( D_{rw} = U_1 A_w Z_2 )</td>
</tr>
<tr>
<td></td>
<td>( D_{qw} = U_1 A_w Z_7 )</td>
</tr>
<tr>
<td>Water-Air</td>
<td>( D_{21} = D_{vw} )</td>
</tr>
<tr>
<td>Air-Soil</td>
<td>( D_{13} = D_{vs} + D_{rs} + D_{os} )</td>
</tr>
<tr>
<td></td>
<td>( D_{vs} = 1/(1/D_{s} + 1/(D_{sw} + D_{sa})) )</td>
</tr>
<tr>
<td></td>
<td>( D_{s} = U_5 A_s Z_1 )</td>
</tr>
<tr>
<td></td>
<td>( D_{sa} = U_7 A_s Z_1 )</td>
</tr>
<tr>
<td></td>
<td>( D_{sw} = U_5 A_s Z_2 )</td>
</tr>
<tr>
<td></td>
<td>( D_{rs} = U_5 A_s Z_2 )</td>
</tr>
<tr>
<td></td>
<td>( D_{os} = U_5 A_s Z_7 )</td>
</tr>
<tr>
<td>Soil-Air</td>
<td>( D_{31} = D_{vs} )</td>
</tr>
<tr>
<td>Water-Sediment</td>
<td>( D_{24} = U_9 A_w Z_5 + U_9 A_S Z_5 )</td>
</tr>
<tr>
<td>Sediment-Water</td>
<td>( D_{42} = U_9 A_w Z_2 + U_9 A_S Z_4 )</td>
</tr>
<tr>
<td>Soil-Water</td>
<td>( D_{32} = U_9 A_s Z_2 + U_9 A_S Z_3 )</td>
</tr>
</tbody>
</table>

### TABLE 1.5.9

**Level III solutions to mass balance equations**

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Mass balance equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>( E_1 + f_1 D_{12} + f_3 D_{13} = f_1 D_{T1} )</td>
</tr>
<tr>
<td>Water</td>
<td>( E_2 + f_1 D_{12} + f_2 D_{14} + f_3 D_{24} = f_1 D_{T2} )</td>
</tr>
<tr>
<td>Sediment</td>
<td>( E_3 + f_1 D_{14} = f_3 D_{T3} )</td>
</tr>
<tr>
<td>where</td>
<td>( f_1 = \frac{D_{14} + f_2 D_{34}}{D_{T4}} )</td>
</tr>
<tr>
<td>Solutions:</td>
<td>( f_2 = \frac{E_1 + J_1 J_3 + E_3 D_{14}/D_{T1} + E_2 D_{12}/D_{T2}}{(D_{T2} - J_1 J_3 - D_{24} D_{34}/D_{T4})} )</td>
</tr>
<tr>
<td></td>
<td>( f_3 = \frac{E_3 + f_2 D_{24}}{D_{T3}} )</td>
</tr>
<tr>
<td></td>
<td>( f_4 = \frac{E_2 + f_3 D_{24}}{D_{T4}} )</td>
</tr>
</tbody>
</table>

where

| \( J_1 = \frac{E_3 D_{14}/D_{T1} + E_3 D_{34}/D_{T3}}{D_{T1} D_{T3}} \) |
| \( J_2 = \frac{D_{24} D_{34}/D_{T4}}{D_{T1}} \) |
| \( J_3 = 1 - D_{14} D_{12}/D_{T1} D_{T3} \) |
| \( J_4 = D_{12} + D_{14} D_{12}/D_{T1} \) |
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 kg/h are simply twice those of 1000 kg/h. Further, if discharge of 1000 kg/h to air causes 500 kg in water and discharge of 1000 kg/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 kg/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 kg/h) responses are given. Also, an illustrative “three discharge” mass balance is given in which a total of 1000 kg/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., °C), boiling point (b.p., °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, Augustijn-Beckers 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, biocen- tration 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, Kow, vapor pressure, and the biocen- tration 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, \( \Delta H_{\text{fus}} \), are generally expressed in kcal/mol or kJ/mol and entropies of fusion, \( \Delta S_{\text{fus}} \), in cal/mol·K (e.u. or entropy unit) or J/mol·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 g/m³ or the equivalent mg/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 (BAF), \( K_{\text{OC}} \), and \( K_{\text{OM}} \) 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 \( 0.693/t_{\frac{1}{2}} \) where \( t_{\frac{1}{2}} \) 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 less-studied 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 $K_{ow}$ 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.
The plot between Henry’s law constant and molar volume (Figure 1.7.4) is more scattered. Figure 1.7.5 shows the often-reported inverse relationship between octanol-water partition coefficient and the supercooled liquid solubility.

The QSPR plots show that an increase in molar volume by 100 cm$^3$/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 $K_{OW}$ by 2.0 units, i.e., a factor of 100.

The plot of log $K_{OW}$ 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).
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, KOW, 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 kg (100 tonnes) of benzene are introduced into the 100,000 km² environment, 99% will partition into air at a concentration of $9.9 \times 10^{-7}$ g/m³ or about 1 µg/m³. The water will contain nearly 1% at a low concentration of 4 µg/m³ or equivalently 4 ng/L. Soils would contain $5 \times 10^{-6}$ µg/g and sediments about $9.7 \times 10^{-6}$ µg/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 $3.14 \times 10^{-5}$ 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 KOC 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 $3.0 \times 10^{-5}$ µg/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 kg/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 kg/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

**FIGURE 1.7.5** Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for mononuclear aromatic hydrocarbons.
Chemical name: Benzene
Fugacity Level I calculations: (six-compartment model)

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 17h half-life, the D value is $1.6 \times 10^9$ mol/Pa·h. For any other process to compete with this would require a value of at least $10^8$ mol/Pa·h. This is achieved by advection ($4 \times 10^8$), 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)

FIGURE 1.7.7 Level II fugacity calculations for benzene in a generic environment.

transport D values (approximately $10^6$ mol/Pa·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.
FIGURE 1.7.8 Level III fugacity calculations for benzene in a generic environment.
The first row describes the condition if 1000 kg/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 kg/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 kg/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 kg/h in water, advective outflow of 134 kg/h and transfer to air of 320 kg/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 \((0.693 \times \text{mass in water})/\text{rate of transfer}\), i.e., \((0.693 \times 133863)/320 = 290\) 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 \(6.7 \times 10^{-4}\) g/m³, or 670 ng/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 kg/h and there is no advection; thus, the primary loss mechanism is transfer to air \((T_{31})\) at a rate of 905 kg/h, with a relatively minor 10 kg/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 \(3.75 \times 10^{-3}\) g/m³ or \(2.5 \times 10^{-3}\) µg/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 kg/h to air, 300 kg/h to water, and 100 kg/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 kg/h. This is 0.6 of the first (air emission) rate of 803 kg/h, i.e., 482 kg/h, plus 0.3 of the second (water emission) rate of 257 kg/h, i.e., 77 kg/h and 0.1 of the third (soil emission) rate of 729 kg/h, i.e., 73 kg yielding a total of \((482 + 77 + 73)\) or 632 kg/h. It is also apparent that the amount in the air of 15500 kg causing a concentration of \(0.155\) µg/m³ is attributable to emissions to air \((0.6 \times 0.197\) or 0.118 µg/m³), emissions to water \((0.3 \times 0.063\) or 0.019 µg/m³) and emissions to soil \((0.1 \times 0.179\) or 0.018 µg/m³). The concentration in water of \(2.0 \times 10^{-3}\) g/m³ or 202 µg/m³ is largely attributable to the discharges to water, which alone cause \(0.3 \times 669\) or 200 µg/m³. Although more is emitted to air, it contributes less than 1 µg/m³ to the water with soil emissions accounting for about 1 µg/m³. 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 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 kg is thus largely controlled by the discharges to water, which account for \((0.3 \times 133863)\) or 40,000 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 pKₐ 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.
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 cm$^3$/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 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 cm$^3$/mol (i.e., a factor of 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 K$_{OW}$ data in Figure 1.7.12 show that the chlorophenols and alkylphenols differ in properties, there being more uncertainty about the K$_{OW}$ 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 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 $H$ lie between –0.1 to –0, i.e., H lies between 0.8 and 0.08, and the resulting air-water partition coefficient K$_{AW}$ or $H/RT$ thus lies between $3 \times 10^{-4}$ and $3 \times 10^{-5}$.

Figure 1.7.14, the plot of log K$_{OW}$ 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 K$_{OW}$ 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 K$_{OW}$ increases by only about 0.36 log units. The slope of the log K$_{OW}$ 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 K$_{OW}$ can
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 1.7.10** 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.
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 kg/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...
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 kg (100 tonnes) of pentachlorophenol (PCP) are introduced into the 100,000 km² 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 kg/h results in an overall fugacity of $3.43 \times 10^{-8}$ 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 kg/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 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 $10^{10}$ mol/Pa·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

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 kg/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

![Diagram of fugacity calculations](image)

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Half-life (h)</th>
<th>Reaction D Value (mol/Pa.h)</th>
<th>Advection D Value (mol/Pa.h)</th>
<th>Concentration (mol/m³)</th>
<th>Reaction Removal (kg/h)</th>
<th>Advection Removal (kg/h)</th>
<th>Total Removal (%)</th>
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</thead>
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<td>4.34E-07</td>
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<td>2.31E+01</td>
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<td>9.36E+01</td>
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<tr>
<td>Suspended sediment (5)</td>
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<td>-</td>
<td>-</td>
<td>5.99E-03</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Biota (6)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2.43E-03</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Fugacity, f = 3.43E-08 Pa  
Total amount, M = 8.91E+06 mol  
Total amount = 2.37E+06 kg  
Total reaction D value, D_R = 1.06E+11 mol/Pa.h  
Total advection D value, D_A = 2.94E+09 mol/Pa.h  
Total D value, D_T = 1.09E+11 mol/Pa.h  
Total loss by reaction = 9.72E+02 kg/h  
Total loss by advection = 2.78E+01 kg/h  
Total loss = 1.00E+03 kg/h  
Reaction residence time, t_R = 2.44E+03 h  
Advection residence time, t_A = 8.53E+04 h  
Overall residence time, t_O = 2.37E+03 h

FIGURE 1.7.16 Level II fugacity calculations for PCP at data determination pH of 5.1.

water (T_{12}) is about 54 kg/h and that from air to soil (T_{13}) 206 kg/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 kg/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 kg/h in water, advective outflow of 392 kg/h and transfer to air (T_{21}) of 2.90 kg/h with
substantial loss of 128 kg/h to sediment. The amount in the water is 392,200 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 

\[
\frac{0.693 \times \text{mass in water}}{\text{rate of transfer}} = \frac{0.693 \times 392,200}{2.90} = 93700 \text{ h.}
\]

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 × 10⁻³ g/m³ or 1.96 µg/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 kg/h and there is no advection; thus, the other loss mechanism is transfer to air (T₁) at a rate of 0.11 kg/h, with a relatively minor 0.8 kg/h to water by run-off. The soil concentration of 0.136 g/m³ is controlled almost entirely by the rate at which the PCP reacts.

**FIGURE 1.7.17** Level I 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.

**FIGURE 1.7.18** Level II fugacity calculations for PCP at environmental pH of 7.

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

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Half-life h</th>
<th>Reaction D Value</th>
<th>Advection D Value</th>
<th>Concentration mol/m³</th>
<th>Loss Reaction kg/h</th>
<th>Loss Advection kg/h</th>
<th>Total Removal %</th>
</tr>
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<tbody>
<tr>
<td>Air (1)</td>
<td>550</td>
<td>5.08E+07</td>
<td>4.03E+08</td>
<td>3.59E-12</td>
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<td>Water (2)</td>
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<td>1.41E+11</td>
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<td>4.20E+02</td>
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<td>Soil (3)</td>
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<td>Bottom sediment (4)</td>
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<td>7.05E+08</td>
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<td>Suspended sediment (5)</td>
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<td>6.32E-04</td>
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</tbody>
</table>

- **Fugacity, f:** 8.89E-09 Pa
- **Total amount, M:** 3.54E+06 mol
- **Total amount:** 9.44E+05 kg
- **Total reaction D value, D_R:** 2.80E+11 mol/Pa.h
- **Total advection D value, D_A:** 1.41E+11 mol/Pa.h
- **Total D value, D_T:** 4.21E+11 mol/Pa.h
- **Total loss by reaction:** 6.65E+02 kg/h
- **Total loss by advection:** 3.35E+02 kg/h
- **Total loss:** 1.00E+03 kg/h
- **Reaction residence time, t_R:** 1.42E+03 h
- **Advection residence time, t_A:** 2.82E+03 h
- **Overall residence time, t_O:** 9.44E+02 h
Chemical name: Pentachlorophenol
Fugacity Level III calculations: (four-compartment model) at data pH of 5.1

**FIGURE 1.7.19** Level III fugacity calculations for PCP at pH of 5.1.
The final scenario is a combination of discharges, 50 kg/h to air, 250 kg/h to water, and 700 kg/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 kg/h. This is 0.05 of the first (air emission) rate of 82.9 kg/h, i.e., 4.14 kg/h, plus 0.25 of the second (water emission) rate of 0.24 kg/h, i.e., 0.06 kg/h and 0.7 of the third (soil emission) rate of 0.0094 kg/h, i.e., 0.0066 kg/h yielding a total of (4.14 + 0.06 + 0.0066) or 4.21 kg/h. It is also apparent that the amount in the air of 3342 kg causing a concentration of $3.342 \times 10^{-8}$ g/m³ or 33 ng/m³ is attributable to emissions to air (0.05 × 658 or 33 ng/m³), emissions to water (0.25 × 1.9 or 0.5 ng/m³) and emissions to soil (0.7 × 0.0743 or 0.052 µg/m³). The concentration in water of $4.97 \times 10^{-4}$ g/m³, or 497 ng/L, is largely attributable to the discharges to water, which alone cause $0.25 \times 1.96 \times 10^{-3}$ g/m³ or $4.9 \times 10^{-4}$ g/m³ or 490 µg/m³, or 490 ng/L. Although more is emitted to soil, it contributes only about 1.1 µg/m³ to the water with air emissions accounting for about 5.27 µg/m³. 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 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 $2.04 \times 10^6$ 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 µPa) 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: Pentachlorophenol
Fugacity Level III calculations: (four-compartment model) at environmental pH of 7

![Diagram of four-compartment model](image)

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

### Phase Properties and Rates:

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Bulk Z (mol/l)</th>
<th>Half-life (h)</th>
<th>Reaction (Advection) D Value (mol/l·h)</th>
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### Emission Scenarios:

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<th>E3</th>
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<th>W1</th>
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<th>Total Amount (kg)</th>
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<td>6.940E+00</td>
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<th>Emission Scenario</th>
<th>E1</th>
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<th>E3</th>
<th>R1</th>
<th>R2</th>
<th>R3</th>
<th>R4</th>
<th>T12</th>
<th>T21</th>
<th>T22</th>
<th>T31</th>
<th>T32</th>
<th>T42</th>
<th>Intermedia Rate of Transport (kg/h)</th>
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<tbody>
<tr>
<td>(Air Only)</td>
<td>1000</td>
<td>0</td>
<td>0</td>
<td>6.656E+00</td>
<td>6.666E-02</td>
<td>8.21E+02</td>
<td>2.618E-01</td>
<td>9.476E+01</td>
<td>7.566E-03</td>
<td>6.476E-02</td>
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<td>2.517E+00</td>
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<td>(Water Only)</td>
<td>0</td>
<td>1000</td>
<td>0</td>
<td>4.197E-04</td>
<td>5.561E+02</td>
<td>5.19E-02</td>
<td>2.154E+00</td>
<td>3.331E-03</td>
<td>4.413E+02</td>
<td>3.467E-01</td>
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<td>(Soil Only)</td>
<td>0</td>
<td>0</td>
<td>1000</td>
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<td>6.490E-02</td>
<td>1.318E-01</td>
<td>1.036E-02</td>
<td>1.245E-01</td>
<td>1.855E-03</td>
<td>1.114E+00</td>
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<td>A+W+S</td>
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<td>250</td>
<td>700</td>
<td>3.387E-01</td>
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<td>4.314E+01</td>
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</table>
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.

### FIGURE 1.7.22 Level III fugacity distributions of PCP for four emission scenarios at pH of 7.

<table>
<thead>
<tr>
<th>Emission to Air Only</th>
<th>Emission to Water Only</th>
<th>Emission to Soil Only</th>
<th>Emission to Air, Water and Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>E&lt;sub&gt;1&lt;/sub&gt; = 1000 kg/h</td>
<td>E&lt;sub&gt;1&lt;/sub&gt; = 0 kg/h</td>
<td>E&lt;sub&gt;1&lt;/sub&gt; = 0 kg/h</td>
<td>E&lt;sub&gt;1&lt;/sub&gt; = 50 kg/h</td>
</tr>
<tr>
<td>E&lt;sub&gt;2&lt;/sub&gt; = 0 kg/h</td>
<td>E&lt;sub&gt;2&lt;/sub&gt; = 1000 kg/h</td>
<td>E&lt;sub&gt;2&lt;/sub&gt; = 0 kg/h</td>
<td>E&lt;sub&gt;2&lt;/sub&gt; = 250 kg/h</td>
</tr>
<tr>
<td>E&lt;sub&gt;3&lt;/sub&gt; = 0 kg/h</td>
<td>E&lt;sub&gt;3&lt;/sub&gt; = 0 kg/h</td>
<td>E&lt;sub&gt;3&lt;/sub&gt; = 1000 kg/h</td>
<td>E&lt;sub&gt;3&lt;/sub&gt; = 700 kg/h</td>
</tr>
</tbody>
</table>

Overall residence time:
- E<sub>1</sub>: 2.07E+03 h
- E<sub>2</sub>: 4.59E+02 h
- E<sub>3</sub>: 2.39E+03 h
- E<sub>4</sub>: 1.89E+03 h

**Distribution of mass:**
- Air: 0.10%
- Soil: 97.09%
- Water: 2.85%

**Distribution of removal rates:**
- Sediment: 0.02%
- Water: 96.19%
- Soil: 99.43%

**Legend**
- Reaction
- Advection
1.8 REFERENCES


Introduction


Sangster, J. (1993) LOGKOW databank. Sangster Research Laboratory, Montreal, Quebec, Canada.


Introduction

# 2 Aliphatic and Cyclic Hydrocarbons

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### Alkenes

<table>
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<td>2-Methylpropene</td>
<td>270</td>
</tr>
<tr>
<td>1-Butene</td>
<td>273</td>
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<tr>
<td>2-Methyl-1-butene</td>
<td>276</td>
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<td>3-Methyl-1-butene</td>
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### Dienes

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<td>2-Methyl-1,3-butadiene (Isoprene)</td>
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<td>1,4-Pentadiene</td>
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<td>1,5-Hexadiene</td>
<td>334</td>
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<td>1,6-Heptadiene</td>
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### Alkynes

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<td>1-Hexyne</td>
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<td>1-Heptyne</td>
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<td>1-Octyne</td>
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<td>1-Nonyne</td>
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### Cycloalkenes

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<td>Cyclooctene</td>
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<td>Cycloheptatriene</td>
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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: C\textsubscript{4}H\textsubscript{10}
Molecular Weight: 58.122
Melting Point (°C):
\[ -159.4 \quad \text{(Weast 1984; Lide 2003)} \]
Boiling Point (°C):
\[ -11.73 \quad \text{(Lide 2003)} \]
Density (g/cm\textsuperscript{3} at 20°C):
\[ 0.5490 \quad \text{(Weast 1984)} \]
\[ 0.5571, 0.5509 \quad \text{(20°C, 25°C, Riddick et al. 1986)} \]
Molar Volume (cm\textsuperscript{3}/mol):
\[ 105.9 \quad \text{(calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)} \]
\[ 96.2 \quad \text{(calculated-Le Bas method at normal boiling point)} \]
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
\[ 19.121, 21.297 \quad \text{(25°C, bp, Riddick et al. 1986)} \]
Enthalpy of Fusion, $\Delta H_fus$ (kJ/mol):
\[ 4.540 \quad \text{(Dreisbach 1959; Riddick et al. 1986)} \]
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
\[ 48.9 \quad \text{(shake flask-GC at atmospheric pressure, McAuliffe 1963, 1966)} \]
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
\[ 101783* \quad \text{(-11.609°C, static method-manometer, measured range –85.5 to –11.609°C, Aston et al. 1940)} \]
\[ 101325* \quad \text{(-11.7°C, summary of literature data, temp range –109.2 to –11.7°C, Stull 1947)} \]
\[ 348100 \quad \text{(calculated from determined expthl. data, Dreisbach 1959)} \]
\[ \log(P/\text{mmHg}) = 6.74808 - 882.80/(240.0 + t/°C); \text{temp range -75 to 30°C (Antoine eq. for liquid state, Dreisbach 1959)} \]
\[ 357000 \quad \text{(interpolated-Antoine eq., temp range -86.57 to 18.88°C, Zwolinski & Wilhoit 1971)} \]
\[ \log(P/\text{mmHg}) = 6.91048 - 946.35/(246.68 + t/°C); \text{temp range -86.57 to 18.88°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]
\[ \log(P/\text{mmHg}) = [-0.2185 \times 5084.4/(T/K)] + 7.250; \text{temp range -115 to -34°C (Antoine eq., Weast 1972–73)} \]
\[ \log(P/\text{mmHg}) = [-0.2185 \times 5416.2/(T/K)] + 7.349085; \text{temp range -109.5 to 137.5°C (Antoine eq., Weast 1972–73)} \]
\[ 312486, 313702* \quad \text{(21.07, 21.22°C, vapor-liquid equilibrium, measured range 4.580–71.17°C, Steele et al. 1976)} \]
\[ 356600 \quad \text{(extrapolated-Antoine eq., temp range ~87 to 7°C, Dean 1985, 1992)} \]
\[ \log(P/\text{mmHg}) = 6.90148 - 946.35/(246.68 + t/°C); \text{temp range -87 to 7°C (Antoine eq., Dean 1985, 1992)} \]
\[ \log(P/\text{kPa}) = 6.00272 - 947.54/(248.87 + t/°C); \text{temp range not specified (Antoine eq., Riddick et al. 1986)} \]
\[ 351130 \quad \text{(interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)} \]
log \( P \) (kPa) = 6.03538 – 946.35/(–26.47 + T/K); temp range 186–280 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log \( P \) (kPa) = 7.83572 – 1470.08/(3.99 + T/K); temp range 121–187 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( P \) (kPa) = 5.93028 – 907.164/(–30.14 + T/K); temp range 263–306 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log \( P \) (kPa) = 6.26924 – 1102.296/(–2.12 + T/K); temp range 301–366 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log \( P \) (kPa) = 6.95371 – 1648.648/(77.939 + T/K); temp range 361–408 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log \( P \) (mmHg) = 31.2541 – 1.9532 × 10^3/(T/K) – 8.806·log (T/K) + 8.9246 × 10–11·(T/K) + 5.7501 × 10–6·(T/K)^2; temp range 114–408 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):

118640 (converted from 1/K_AW = C_W/C_A reported as exptl., Hine & Mookerjee 1975)

100980, 22090 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

120000 (calculated-P/C, Mackay & Shiue 1981)

116700 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

2.76 (shake flask-GC, Leo et al. 1975)

2.76 (recommended, Sangster 1993)

2.76 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \) and Half-Lives, \( t_\text{1/2} \):

Volatileization:

Photolysis:

Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression

see reference:

\( k_{OH} \) (exptl) = 1.42 × 10^{12} cm^3 mol^{-1} s^{-1}, \( k_{OH} \) (calc) = 1.31 × 10^{12} cm^3 mol^{-1} s^{-1} at 297 K, measured range 297–499 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

\( k_{OH} \) = 1.28 × 10^{9} L mol^{-1} s^{-1} at 300 K (Greiner 1967; quoted, Altshuller & Bufalini 1971)

\( k_{OH} \) = (2.52 ± 0.05) × 10^{12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

\( k_{O3} \) = 2.0 × 10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K, temp range 298–323 K (Atkinson & Carter 1984)

\( k_{OH} \) = (2.29 ± 0.06) × 10^{12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

\( k_{OH} \) = (2.34 ± 0.33) × 10^{-12} cm^3 molecule^{-1} s^{-1} at (24.6 ± 0.4)°C (Edney et al. 1986)

\( k_{OH} \) = 2.34 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

\( k_{OH} \) = 2.34 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, \( k_{NO3} \) = 9.7 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (recommended, Atkinson 1990)

\( k_{NO3} \) = (1.10 ± 0.2) × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–523 K, atmospheric \( t_\text{1/2} \) = 1750 h during the night at room temp. (discharge flow system, Bagley et al. 1990)

\( k_{OH} \) = 7.38 × 10^{-13} cm^3 molecule^{-1} s^{-1}, \( k_{NO3} \) = 6.50 × 10^{-17} cm^3 molecule^{-1} s^{-1} (Sabljic & Güsten 1990)

\( k_{NO3} \) = 9.8 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1991)

\( k_{OH} \) = 2.34 × 10^{-12} cm^3 molecule^{-1} s^{-1} and an estimated lifetime was 59 h (Altshuller 1991)

\( k_{NO3} \) (exptl) = 9.8 × 10^{-17} cm^3 molecule^{-1} s^{-1}, \( k_{NO3} \) (recommended) = 9.9 × 10^{-17} cm^3 molecule^{-1} s^{-1}, \( k_{NO3} \) (calc) = 7.90 × 10^{-17} cm^3 molecule^{-1} s^{-1}, at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

\( k_{OH} \) = 2.19 × 10^{-12} cm^3 molecule^{-1} s^{-1}, \( k_{NO3} \) = 10.6 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: atmospheric t₁/₂ = 1750 h due to reaction with NO₃ radical during the night at room temp., and t₁/₂ = 82 h for reaction with OH radical (Bagley et al. 1990);
atmospheric lifetime was estimated to be 59 h, based on a photooxidation rate constant k = 2.34 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ in summer daylight with OH radical (Altshuller 1991).

**TABLE 2.1.1.1.1**
Reported vapor pressures of isobutane (2-methylpropane) at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>–85.5</td>
<td>1516</td>
<td>–109.2</td>
<td>133.3</td>
<td>4.580</td>
<td>183196</td>
</tr>
<tr>
<td>–71.704</td>
<td>4261</td>
<td>–91.1</td>
<td>666.6</td>
<td>4.620</td>
<td>185019</td>
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<tr>
<td>–56.431</td>
<td>11579</td>
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<td>–44.107</td>
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</table>

**FIGURE 2.1.1.1.1** 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: C₅H₁₂
Molecular Weight: 72.149
Melting Point (°C):
-16.4 (Lide 2003)
Boiling Point (°C):
9.503 (Dreisbach 1959; Stephenson & Malanowski 1987)
9.48 (Lide 2003)
Density (g/cm³ at 20°C):
0.5910, 0.5852 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
122.10 (20°C, calculated-density, McAuliffe 1966; Wang et al. 1992)
117.6 (20°C, Stephenson & Malanowski 1987)
118.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
Enthalpy of Fusion, ∆Hfus (kJ/mol):
3.255 (Dreisbach 1959; Chickos et al. 1999)
3.146 (Riddick et al. 1986)
Entropy of Fusion, ∆Sfus (J/mol K):
12.69 (exptl., Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
33.2 (shake flask-GC at 1 atmospheric pressure, McAuliffe 1966)
Vapor Pressure (Pa at 25°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°C, Stull 1947)
171350 (calculated from determined data, Dreisbach 1959)
log (P/mmHg) = 6.73812 – 950.84/(237.0 + t°C); temp range -60 to 55°C (Antoine eq. for liquid state, Dreisbach 1959)
171586* (derived from compiled data, temp range -13.729 to 29.914°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.2034 – 1020.7/(–43.15 + T/K); temp range 223–256 K (Antoine eq-I., Stephenson & Malanowski 1987)
log (P/mmHg) = 6.60427 – 883.42/(227.782 + t°C); temp range -13.729 to 29.914°C (Antoine eq., liquid, Zwolinski & Wilhoit 1971)
log (P/mmHg) = (–0.2185 × 5648.6/(T/K)) + 7.263947; temp range -102 to 152.5°C (Antoine eq., Weast 1972–73)
169019* (24.56°C, ebulliometry, measured range -5.128 to 40°C, Osborn & Douslin 1974)
log (P/mmHg) = 6.60427 – 883.42/(227.782 + t°C); temp range -14 to 29°C (Antoine eq., Dean 1985, 1992)
171300 (selected, Riddick et al. 1986)
log (P/kPa) = 6.89316 – 938.234/(235.249 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
171520, 171450 (interpolated-Antoine eq.-III and IV, Stephenson & Malanowski 1987)
log (P/kPa) = 6.3283 – 1020.7/(-43.15 + T/K); temp range 223–256 K (Antoine eq-I., Stephenson & Malanowski 1987)
log \( \frac{P}{kPa} \) = 7.07825 – 1372.459/(–8.39 + T/K); temp range 223–256 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( \frac{P}{kPa} \) = 5.76532 – 900.545/(–43.111 + T/K); temp range 268–313 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log \( \frac{P}{kPa} \) = 5.83935 – 937.641/(–38.071 + T/K); temp range 257–315 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log \( \frac{P}{kPa} \) = 6.08953 – 1080.237/(–17.896 + T/K); temp range 312–385 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log \( \frac{P}{kPa} \) = 7.26795 – 2114.713/(128.175 + T/K); temp range 382–433 K (Antoine eq-VI, Stephenson & Malanowski 1987)

\[ \log (P/mmHg) = 26.6662 – 1.9307 \times 10^3/(T/K) – 7.0448 \cdot \log (T/K) + 7.4104 \times 10^{-9} \cdot (T/K)^2; \]
\[ \text{temp range 257–434 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa m^3/mol at 25°C):

221000 (calculated as \( I/K_{AW} \ C_W/C_A \) 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, \( \log K_{OW} \):

3.11 (shake flask-GC, Leo et al. 1975; Leo et al. 1971; Hansch & Leo 1979)
2.95, 3.41, 3.22 (calculated-fragment const., Rekker 1977)
3.30, 3.08 (calculated-MO, calculated-\( \pi \) const., Bodor et al. 1989)
3.11 (recommended, Sangster 1989, 1993)
2.98 (calculated-V_M, Wang et al. 1992)
3.11 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{OC} \):

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO3 radical and \( k_{O3} \) with O3, or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[ k_{OH}^*(\text{exptl}) = 6.50 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, k_{OH}(\text{calc}) = 5.27 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ at 298 K, measured range 298–493 K} \text{ (flash photolysis-kinetic spectroscopy, Greiner 1970)} \]

\[ k_{OH}(\text{exptl}) = 6.50 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, k_{OH}(\text{calc}) = 5.37 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ at 298 K} \text{ (Greiner 1970)} \]

\[ k_{O3P} = 5.50 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O(3P) atom at room temp. (Herron & Huie 1973)} \]

\[ k_{OH} = (1.04 \pm 0.17) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 300 K} \text{ (relative rate method, Darnall et al. 1978)} \]

\[ k_{OH} = 9.30 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson et al. 1979)} \]

\[ k_{OH} = 9.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Winer et al. 1979)} \]

\[ k_{OH}^* = 8.49 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989, 1990, 1991)} \]

\[ k_{OH}^* = 8.48 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1997)} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A[1 - \Phi/(T/K)] \quad (5) \\
\end{align*}
\]

where \( \log A = a + b(T/K) + c(T/K)^2 \)

Stull 1947
Zwolinski & Wilhoit 1971
Osborn & Douslin 1974

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<th>(T/°C)</th>
<th>(P/Pa)</th>
<th>(T/°C)</th>
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bp/°C 9.478
mp/°C –16.4 °C

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<td>250</td>
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Antoine eq. 1 P/mmHg
A 7.0344 199146
B 220.7 499176
C 230.0 599187

Cox eq. 2 P/mmHg
A 7.0344 199146
B 220.7 499176
C 230.0 599187

C 227.782

FIGURE 2.1.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2,2-dimethylpropane.
2.1.1.3  

**n-Butane**

---

**Common Name:** n-Butane  
**Synonym:** 1-butane  
**Chemical Name:** n-butane  
**CAS Registry No:** 106-97-8  
**Molecular Formula:** C\(_4\)H\(_8\)  
**Molecular Weight:** 58.122  
**Melting Point (°C):**  
–138.3 (Lide 2003)  
**Boiling Point (°C):**  
–0.50 (Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)  
**Density (g/cm\(^3\) at 20°C):**  
0.5788, 0.5730 (20°C, 25°C, Dreisbach 1959)  
0.5786, 0.5729 (20°C, 25°C, Riddick et al. 1986)  
**Molar Volume (cm\(^3\)/mol):**  
100.45, 101.45 (20°C, 25°C, calculated-density)  
96.2 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):**  
21.066, 22.393 (25°C, bp, Riddick et al. 1986)  
**Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):**  
4.393 (Parks & Huffman 1931)  
4.661 (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)  
**Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):**  
34.56 (exptl., Chickos et al. 1999)  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m\(^3\) or mg/L at 25°C):**  
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°C or as indicated and reported temperature dependence equations):**  
288200 (extrapolated-Antoine eq. regression, temp range ~101.5 to ~0.5°C, Stull 1947)  
243050 (calculated from determined data, Dreisbach 1959)  
\[\log (P/mmHg) = 6.83029 – 945.9/(240.0 + t/°C); \text{temp range ~60 to 30°C (Antoine eq. for liquid state, Dreisbach 1959)}\]  
242647 (derived from compiled data, temp range ~77.62 to 18.88°C, Zwolinski & Wilhoit 1971)  
\[\log (P/mmHg) = 6.80896 – 935.56/(238.73 + t/°C); \text{temp range ~77.62 to 18.88°C (Antoine eq., Zwolinski & Wilhoit 1971)}\]  
242840 (extrapolated-Antoine eq., temp range ~77 to 19°C, Dean 1985, 1992)  
\[\log (P/mmHg) = 6.80896 – 935.86/(238.73 + t/°C); \text{temp range ~77 to 19°C (Antoine eq., Dean 1985, 1992)}\]  
243000 (lit. average, Riddick et al. 1986)  
\[\log (P/kPa) = 5.93266 – 935.773/(238.789 + t/°C); \text{temp range not specified (Antoine eq., Riddick et al. 1986)}\]  
242810 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)  
\[\log (P/kPa) = 5.93386 – 935.86/(–34.52 + T/K); \text{temp range 195–292 K (Antoine eq.-I, Stephenson & Malanowski 1987)}\]  
\[\log (P/kPa) = 7.3327 – 1409.73/(T/K); \text{temp range 135–213 K (Antoine eq.-II, Stephenson & Malanowski 1987)}\]  
\[\log (P/kPa) = 6.07512 – 1007.247/(–25.272 + T/K); \text{temp range 273–321 K (Antoine eq.-III, Stephenson & Malanowski 1987)}\]
Aliphatic and Cyclic Hydrocarbons

\[
\log \left( \frac{P}{\text{kPa}} \right) = 6.32267 - 1161.1/(-3.107 + T/\text{K}) \quad \text{temp range 316-383 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
\log \left( \frac{P}{\text{kPa}} \right) = 7.04942 - 1770.348/(84.979 + T/\text{K}) \quad \text{temp range 375-425 K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]

\[
\log \left( \frac{P}{\text{mmHg}} \right) = 27.0441 - 1.9049 \times 10^3/(T/\text{K}) - 7.1805 \cdot \log (T/\text{K}) - 6.6845 \times 10^{-11} \cdot (T/\text{K})^2 \quad \text{temp range 135-425 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C):

- 94240 (calculated-1/K_{AW}, C_w/C_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 K_{OW}:

- 2.89 (shake flask-GC, Leo et al. 1975)
- 2.89 (concen. 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 K_{OA}:

- 1.53 (calculated-measured \gamma^* in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_\text{1/2}:

Vaporization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[
\begin{align*}
\text{k}_{\text{OH}} &= 9.8 \times 10^{-24} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 298-323 \text{ K (Schubert & Pease 1956)} \\
\text{k}_{\text{OH}} &= 3.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O(3P) atom (Herron & Huie 1973)} \\
\text{k}_{\text{OH}} &= 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Atkinson et al. 1979)} \\
\text{k}_{\text{OH}}(\text{exptl}) &= (2.57 - 4.22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{k}_{\text{OH}}(\text{calc}) = 2.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 298-495 \text{ K (flash photolysis-kinetic spectroscopy, Greiner 1970)} \\
\text{k}_{\text{OH}} &= 1.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with atmospheric } t_{\text{OH}} = 2.4 \text{ to } 24 \text{ h at } 300 \text{ K (Darnall et al. 1976)} \\
\text{k}_{\text{OH}} &= 1.8 \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \text{ in polluted atmosphere at } 305 \pm 2 \text{ K (relative rate method, Lloyd et al. 1976)} \\
\text{k}_{\text{OH}} &= 3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 0.11 \text{ d}^{-1} \text{ for the reaction with OH radical and an average OH concn of } 1.2 \times 10^6 \text{ molecules/cm}^3 \text{ (Zafonte & Bonamassa 1977)} \\
\text{k}_{\text{OH}}(\text{exptl}) &= (2.57 - 4.22) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{k}_{\text{OH}}(\text{calc}) = 2.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at atmospheric pressure and } 300 \text{ K (Darnall et al. 1978)} \\
\text{k}_{\text{OH}} &= 2.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \pm 2 \text{ K (relative rate method, Atkinson et al. 1982a, 1984c)} \\
\text{k}_{\text{O3}} &< 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } < 6 \times 10^{-7} \text{ d}^{-1}, \text{k}_{\text{OH}} = 2.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 0.2 \text{ d}^{-1} \text{ and } \text{k}_{\text{NO3}} = 3.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 0.0007 \text{ d}^{-1} \text{ (Atkinson & Carter 1984; Atkinson 1985)} \\
\text{k}_{\text{OH}} &= 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)} \\
\text{k}_{\text{OH}}(\text{exptl}) &= 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, } \text{k}_{\text{NO3}} = 6.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (Atkinson 1990; Altshuller 1991).}
\end{align*}
\]
k_{NO_3}^* = (0.45 \pm 0.06) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 298–523 \text{ K, atmospheric } t_{1/2} = 4300 \text{ 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)

k_{NO_3} = (\leq 2.0 – 6.6) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296–298 \text{ K (Atkinson 1991)}

k_{NO_3}(\text{exptl}) = 6.70 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3}(\text{recommended}) = 4.3 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (relative rate method, Aschmann & Atkinson 1995)}

k_{OH}^* = 2.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3}^* = 4.59 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)}

k_{OH} = 2.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, measured range } 230–400 \text{ K (relative rate method, DeMore & Bayes 1999)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 6.5 \text{ h in ambient air based on reaction with OH radicals at } 300 \text{ K (Doyle et al. 1975)}$;

photoysis $t_{1/2} = 2.4 \text{ to } 24 \text{ h (Darnall et al. 1976)}$;

atmospheric lifetimes $\tau(\text{calc}) = 4 \times 10^7 \text{ h for reaction with O}_3, \tau = 107 \text{ h with OH radical and } \tau = 32150 \text{ h with NO}_3 \text{ radical based on reaction rate constants and environmental concentrations of OH, NO}_3 \text{ radicals and O}_3 \text{ in the gas phase (Atkinson & Carter 1984)}$;

atmospheric lifetimes $\tau(\text{calc}) = 222 \text{ h for the reaction with OH radical, } \tau = 4 \times 10^7 \text{ h with O}_3 \text{ and } \tau = 32150 \text{ h with NO}_3 \text{ radical based on the rate constants and environmental concentrations of OH, NO}_3 \text{ radicals and O}_3 \text{ in the gas phase (Atkinson 1985)}$;

atmospheric $t_{1/2} = 4300 \text{ h due to reaction with NO}_3 \text{ during the night at room temp., and } t_{1/2} = 77 \text{ h for reaction with OH radical (Bagley et al. 1990)}$;

atmospheric lifetime $\tau \sim 54 \text{ h based on a photooxidation reaction rate constant of } 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with OH radicals during summer daylight hours (Altshuller 1991)}$. 
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: C₅H₁₂; CH₃CH(CH₃)CH₂CH₃
Molecular Weight: 72.149
Melting Point (°C): 
-159.77 (Lide 2003)
Boiling Point (°C): 27.875
  27.88 (Lide 2003)
Density (g/cm³ at 20°C): 
0.6197, 0.6146 (20°C, 25°C, Dreisbach 1959)
0.6193, 0.6142 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol): 
116.5, 117.47 (20°C, 25°C, calculated-density)
118.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol): 
5.1505 (Dreisbach 1959, Riddick et al. 1986)
5.13 (Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K): 
45.23, 43.35 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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*  (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)
72.4; 49.6, 55.2  (0, 25°C, 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°C, Shaw 1989)
52.11*  (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–323.2 K, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
82790  (22.04°C, Schumann et al. 1942)
\[ \log (P/\text{mmHg}) = 6.87372 - 1075.816/(233.259 + t/°C) \]  temp range 16.291–28.587°C (Antoine eq. from exptl. data, manometer, Willingham et al. 1945)
99550*  (Antoine eq. regression, temp range –82.9 to 27.8°C, Stull 1947)
91740  (calculated from determined data, Dreisbach 1959)
\[ \log (P/\text{mmHg}) = 6.78967 - 1020.012/(223.097 + t/°C) \]  temp range –45 to 75°C (Antoine eq. for liquid state, Dreisbach 1959)
91646*  (extrapolated-Antoine eq, temp range –67.03 to 49.14°C, Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 6.83315 - 1040.73/(235.455C + t/°C) \]  temp range –67.03 to 49.14°C (Antoine eq., Zwolinski 
& Wilhoit 1971)
\[ \log (P/\text{mmHg}) = [-0.2185 \times 6470.8/(T/K)] + 7.544680; \text{temp range:} –82.9 to 180.3°C, (Antoine eq., Weast 1972–73)
91730, 92100 (interpolated, Antoine equations, Boublik et al. 1984)
log (P/kPa) = 6.04913 – 1081.748/(239.817 + t°C); temp range –56 to 22.4°C (Antoine eq. from reported exptl. data of Schumann et al. 1942, Boublik et al. 1984)
log (P/kPa) = 5.9333 – 1029.602/(234.294 + t°C); temp range 16.29–28.59°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°C, Dean 1985)
log (P/mmHg) = 6.91048 – 946.35/(246.68 + t°C); temp range –87 to 7°C (Antoine eq., Dean 1985, 1992)
91700 (quoted, Riddick et al. 1986)
log (P/kPa) = 5.95805 – 1040.73/(–37.705 + T/K); temp range 216–323 K (Antoine eq-I., Stephenson & Malanowski 1987)
log (P/kPa) = 6.32287 – 1279.08/(–4.481 + T/K); temp range 300–460 K (Antoine eq-II., Stephenson & Malanowski 1987)
log (P/kPa) = 6.39629 – 1325.048/(1.244 + T/K); temp range 320–391 K (Antoine eq-III., Stephenson & Malanowski 1987)
log (P/kPa) = 6.22589 – 1212.803/(–12.958 + T/K); temp range 385–416 K (Antoine eq-IV., Stephenson & Malanowski 1987)
log (P/kPa) = 8.09160 – 3167.07/(233.708 + T/K); temp range 412–460 K (Antoine eq-V., Stephenson & Malanowski 1987)
log (P/mmHg) = 29.2963– 2.1762 × 10 3/(T/K) – 7.883·log (T/K) – 4.6512 × 10–11·(T/K)2; temp range 113–460 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C):
140000 (calculated-P/C, Mackay et al. 1979; Mackay 1981)
138000; 140000, 139000, 134700 (recommended; calculated-P/C, Mackay & Shiу 1981))
138210 (selected, Mills et al. 1982)
138290 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:
2.30 (calculated-π constant, Hansch et al. 1968)
2.41 (calculated-MCI χ, Murray et al. 1975)
2.83 (calculated-molar volume V_m, Wang et al. 1992)
2.4698 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatileization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{oh} for reaction with OH radical, k_{no3} with NO3 radical and k_{oz} with O3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_{oh} = 2.0 × 10^{12} cm^3 mol^{-1} s^{-1} with atmospheric t_o = 2.4–24 h (Lloyd 1976, Darnall et al. 1976)
k_{oh} = (3.78 ± 0.07) × 10^{12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)
k_{oh} = (3.97 ± 0.11) × 10^{12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)
k_{oh} = 3.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)
k_{oh} = 3.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990, 1991; Altshuller 1991)
k_{no3} = (1.60 ± 0.2) × 10^{10} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 298–523 K, atmospheric t_o = 1200 h during the night at room temp. (discharge flow system, Bagley et al. 1990)
k_{oh} = 3.9 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, estimated atmospheric lifetime of 36 h (Altshuller 1991)
k_{NO_3}^{(exptl)} = 1.56 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{NO_3}^{(calc)} = 2.49 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (relative rate method, Aschmann & Atkinson 1995)}

k_{OH} = 3.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{NO_3}^{*} = 1.62 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of $2.0 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976) with atmospheric $t_{1/2} = 2.4–24 \text{ h (Darnall et al. 1976)}$; atmospheric $t_{1/2} = 1200 \text{ h due to reaction with NO}_3 \text{ radical during the night at room temp.}, \text{ and } t_{1/2} = 50 \text{ for reaction with OH radical (Bagley et al. 1990)}$; atmospheric lifetime of $36 \text{ h, based on rate constant of } 3.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
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<tr>
<td>in IUPAC 1989 shake flask-GC/FID IUPAC recommended calc-recommended LLE data</td>
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<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>20</td>
<td>46.9</td>
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<td>72.4</td>
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<td>40</td>
<td>57.7</td>
<td>25</td>
<td>49.6</td>
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<td>70.1</td>
<td>25</td>
<td>48.5</td>
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<td>51</td>
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<tr>
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<td>60</td>
<td>79</td>
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**FIGURE 2.1.1.1.4.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylbutane.
TABLE 2.1.1.4.2
Reported vapor pressures of 2-methylbutane (isopentane) at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>eq.</th>
<th>Willingham et al. 1945</th>
<th>Stull 1947</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
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<td>summary of literature data</td>
<td>selected values</td>
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<tr>
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<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
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<td>22.435</td>
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<td>666.6</td>
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<td>26.773</td>
<td>97608</td>
<td>-57.0</td>
<td>1333</td>
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<td>27.24</td>
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<td>-47.3</td>
<td>2666</td>
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<td>27.673</td>
<td>100700</td>
<td>-36.5</td>
<td>5333</td>
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<tr>
<td>28.16</td>
<td>102402</td>
<td>-29.6</td>
<td>7999</td>
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<tr>
<td>28.587</td>
<td>103922</td>
<td>-20.2</td>
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<tr>
<td>bp/°C</td>
<td>27.852</td>
<td>10.5</td>
<td>53329</td>
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<td>eq. 2</td>
<td>P/mmHg</td>
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<td>101325</td>
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<tr>
<td>A</td>
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<td>mp/°C</td>
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<tr>
<td>B</td>
<td>1020.012</td>
<td>10.53</td>
<td>53329</td>
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<tr>
<td>C</td>
<td>233.097</td>
<td>21.208</td>
<td>79993</td>
</tr>
</tbody>
</table>

FIGURE 2.1.1.4.2 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: C₆H₁₄; CH₃CH(CH₃)₂CH₂CH₃
Molecular Weight: 86.175
Melting Point (°C):
  -99.8 (Lide 2003)
Boiling Point (°C):
  49.73 (Lide 2003)
Density (g/cm³ at 20°C):
  0.6492, 0.6445 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
  132.74, 133.71 (20°C, 25°C, calculated-density)
  140.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHfus (kJ/mol):
  5.791 (Dreisbach 1959; Riddick et al. 1986)
  5.4, 0.28, 0.58 (–146.35, –132.35, –98.95°C, Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
  45.88, 42.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  18.4 (shake flask-GC, McAuliffe 1963, 1966)
  39.4, 23.8 (0, 25°C, 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, Mączyński et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
  43320 (24.47°C, manometer, temp range 15.376–50.529°C, Willingham et al. 1945)
  log (P/mmHg) = 6.75483 – 1081.176/(229.343 + t°C); temp range 15.376–50.529°C (Antoine eq. from exptl. data, manometer, Willingham et al. 1945)
  43480 (Antoine eq. regression, temp range –69.3 to 49.7°C, Stull 1947)
  42570 (25°C, Nicolini & Laffitte 1949)
  42540 (calculated from determined data, Dreisbach 1959; quoted, Hine & Mookerjee 1975)
  log (P/mmHg) = 6.75483 – 1081.176/(229.343 + t°C); temp range –25 to 95°C (Antoine eq. for liquid state, Dreisbach 1959)
  42543 (interpolated-Antoine eq., temp range –41.5 to 72.8°C, Zwolinski & Wilhoit 1971)
  log (P/mmHg) = 6.75483 – 1081.176/(229.343 + t°C); temp range –41.5 to 72.8°C (Antoine eq., Zwolinski & Wilhoit 1971)
  log (P/mmHg) = [–0.2185 × 7271.0/(T/K)] + 7.84130; temp range –69.3 to 49.7°C (Antoine eq., Weast 1972–73)
  42585, 42550 (interpolated-Antoine equations, Boublik et al. 1984)
  log (P/kPa) = 5.88698 – 1085.038/(229.817 + t°C); temp range 15.376–50.53°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
  log (P/kPa) = 5.87001 – 1080.723/(229.842 + t°C); temp range 0–45°C (Antoine eq. from reported exptl. data of Nicolini & Laffitte 1949, Boublik et al. 1984)
log (P/mmHg) = 6.75483 – 1081.176/(229.34 + t/°C); temp range –42 to 73°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 5.87963 – 1081.14/(229.34 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (PL/kPa) = 5.87731 – 1079.789/(–43.978 + T/K); temp range 293–324 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 33.1285 – 2.4527 × 103/(T/K) –9.2016·log (T/K) – 4.7077 × 10–10·(T/K)2; temp range 174–489 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

173000 (calculated-P/C, Mackay & Shiu 1981)
196800 (calculated as 1/KAW/CA, 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 χ, Nirmalakhandan & Speece 1988)
153890 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log KOW:

3.82 (calculated-fragment const., Valvani et al. 1981)
3.25 (calculated-VM, Wang et al. 1992)
3.82 (recommended, Sangster 1993)
3.82 (Hansch et al. 1995)

Octanol/Air Partition Coefficient, log KOA:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Oxidation: rate constant k, for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

kOH = (2.66 ± 0.08) × 10−12 cm³ molecule⁻¹ s⁻¹ at room temp. (relative rate, Atkinson et al. 1984c)

kOH = (2.59 - 6.16) × 10−12 cm³ molecule⁻¹ s⁻¹ at 297–299 K (Atkinson 1985)

kOH* = (2.22 - 0.36) × 10−12 cm³ molecule⁻¹ s⁻¹ at 299 K, measured range 245–328 K (relative rate method, Harris & Kerr 1988; Atkinson 1989)

kOH* = 2.32 × 10−12 cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990)

kOH* = 2.34 × 10−12 cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants or Half-Lives:

Half-Lives in the Environment:
2.1.1.6 2,3-Dimethylbutane

Common Name: 2,3-Dimethylbutane
Synonym: diisopropyl
Chemical Name: 2,3-dimethylbutane
CAS Registry No: 79-29-8
Molecular Formula: C₆H₁₄; CH₃CH(CH₃)CH(CH₃)CH₃
Molecular Weight: 86.175

Melting Point (°C):
-128.10  (Lide 2003)

Boiling Point (°C):
57.93   (Lide 2003)

Density (g/cm³ at 20°C):
0.6616, 0.6570  (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
0.6616   (Weast 1984)

Molar Volume (cm³/mol):
130.25, 131.16  (20°C, 25°C, calculated-density)
140.6  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
29.12, 27.275  (25°C, bp, Dreisbach 1959)
29.125, 27.276  (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, $\Delta H_{ fus}$ (kJ/mol):
0.812  (Dreisbach 1959)
0.7991  (Riddick et al. 1986)
6.43, 2.37, 0.79  (–137.05, –166.15, –127.95°C, Chickos et al. 1999)

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

Fugacity Ratio at 25°C, $F$: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
32.9, 22.5  (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
19.1*  (shake flask-GC, measured range 25–149.5°C, Price 1976)
11.0  (selected, Riddick et al. 1986)
21.0*  (IUPAC tentative value, temp range 0 – 150°C, Shaw 1989a)
18.67*  (calculated-liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Maczyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
28955*  (23.10°C, ebulliometry, measured range: 14.256–58.789°C, Willingham et al. 1945)
log (P/mmHg) = 6.80983 – 1127.187/(228.900 + t°C); temp range 14.256–58.789°C (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)
31204*  (calculated-Antoine eq. regression, temp range –63.6 to 58°C, Stull 1947)
31280  (calculated from determined data, Dreisbach 1959)
log (P/mmHg) = 6.90983 – 1127.187/(228.9 + t°C); temp range –20 to 100°C (Antoine eq. for liquid state, Dreisbach 1959)
31277*  (Antoine eq., temp range –34.9 to 81.3°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.80983 – 1127.187/(228.9 + t°C); temp range –34.9 to 81.3°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 7120.0/(T/K)] + 7.536008; temp range –63.6 to 225.5°C (Antoine eq., Weast 1972–73)
log (P/kPa) = 5.594371 – 1132.099/(229.494 + t/°C); temp range 14.256–58.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/mmHg) = 6.80983 – 1127.83/(228.90 + t/°C); temp range –35 to 81°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 5.93941 – 1129.73/(229.215 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 6.80983 – 1127.83/(228.90 + t/°C); temp range –35 to 81°C (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 33.6319 – 2.5524 × 10^3/(T/K) – 9.3142·log (T/K) + 1.4759 × 10–10·(T/K) + 3.914 × 10–6·(T/K)^2; temp range 145–500 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°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 K_{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 K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_½:

Vaporization:

Photolysis:

Photooxidation: rate constant k, for gas-phase second order rate constants, k_{SH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH}^*(exptl) = 5.16 × 10^{12} cm^3 mol^{-1} s^{-1}, k_{OH}^*(correlated) = 4.49 × 10^{12} cm^3 mol^{-1} s^{-1} at 300 K, measured range 300–498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k_{O3P} = 2.0 × 10^{13} cm^3 molecule^{-1} s^{-1} for the reaction with O(3P) atom at room temp. (Herron & Huie 1973)

k_{OH} = 5.50 × 10^{12} cm^3 molecule^{-1} s^{-1} at room temp. (Atkinson et al. 1979)

k_{OH} = 5.50 × 10^{12} cm^3 molecule^{-1} s^{-1} for reaction with O(3P) atom at room temp. (abstraction mechanism, Gaffney & Levine 1979)

k_{OH} = (5.67 ± 0.29) × 10^{12} cm^3 molecule^{-1} s^{-1} at 300 K (relative rate method, Darnall et al. 1978)

k_{OH} = (6.26 ± 0.06) × 10^{12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k_{NO3} = 4.06 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (relative rate method, Atkinson et al. 1988)

k_{OH}^* = (5.90 - 0.23) × 10^{12} cm^3 molecule^{-1} s^{-1} at 295 K, measured range 247–327 K (relative rate method, Harris & Kerr 1988)

k_{OH} = 6.2 × 10^{12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH} = 6.3 × 10^{12} cm^3 molecule^{-1} s^{-1} with an estimated atmospheric lifetime of 22 h in air during summer daylight (Altshuller 1991)

k_{OH} = 6.30 × 10^{12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 4.06 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)

k_{OH} = 19.0 × 10^{12} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 4.06 × 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (Sabljic & Güsten 1990)

k_{NO3} = (4.04 - 5.34) × 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 K (review, Atkinson 1991)

k_{OH} = 6.3 × 10^{12} cm^3 molecule^{-1} s^{-1} at 298 K, k_{NO3} = 40.6 × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson 1990)
Aliphatic and Cyclic Hydrocarbons

\[ k_{NO_3}^{(\text{expt})} = 4.08 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]
\[ k_{NO_3}^{(\text{recommended})} = 2.55 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]
\[ k_{NO_3}^{(\text{calc})} = 2.55 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (relative rate method, Aschmann & Atkinson 1995)} \]

\[ k_{OH}^{*} = 5.78 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]
\[ k_{NO_3} = 4.40 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of \( 6.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) 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

<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>shake flask-GC</td>
<td>shake flask-GC/FID</td>
<td>IUPAC tentative values</td>
<td>calc-recommended LLE data</td>
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<td>( t/\degree C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
<td>( t/\degree C )</td>
<td>( S/\text{g} \cdot \text{m}^{-3} )</td>
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<td>0</td>
<td>32.9</td>
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<td>25</td>
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</table>

**FIGURE 2.1.1.1.6.1** Logarithm of mole fraction solubility \( (\ln x) \) versus reciprocal temperature for 2,3-dimethylbutane.
TABLE 2.1.1.6.2
Reported vapor pressures of 2,3-dimethylbutane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C\log(T/K)
\end{align*}
\]

Willingham et al. 1945
Stull 1947
Zwolinski & Wilhoit 1971

<table>
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<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<td>14.256</td>
<td>19921</td>
<td>–63.6</td>
<td>133.3</td>
<td>–34.9</td>
<td>1333</td>
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<td>18.044</td>
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<td>57.317</td>
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<td>101325</td>
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<td>26664</td>
</tr>
<tr>
<td>57.79</td>
<td>100693</td>
<td>58.0</td>
<td>101325</td>
<td>21.097</td>
<td>26664</td>
</tr>
<tr>
<td>58.32</td>
<td>102390</td>
<td>mp/°C</td>
<td>–128.2</td>
<td>31.257</td>
<td>39997</td>
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<tr>
<td>58.789</td>
<td>103907</td>
<td>mp/°C</td>
<td>–128.2</td>
<td>31.257</td>
<td>39997</td>
</tr>
</tbody>
</table>

m.p. = 57.93 °C
\[\Delta H_f/(kJ \ mol^{-1}) = \text{at } 25°C \text{ at bp} \]

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<th>bp/°C</th>
<th>P/mmHg</th>
<th>mp/°C</th>
<th>P/mmHg</th>
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<td>19998</td>
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<td>50.682</td>
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<td>55.404</td>
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<td>56.283</td>
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<td>57.568</td>
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</tbody>
</table>

FIGURE 2.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylbutane.
2.1.1.1.7 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: C7H16; CH₃CH(CH₃)₂CH(CH₃)₂
Molecular Weight: 100.202
Melting Point (°C): -24.6 (Lide 2003)
Boiling Point (°C): 80.86 (Lide 2003)
Density (g/cm³ at 20°C):
0.6901, 0.6859 (20°C, 25°C, Dreisbach 1959)
0.6901 (Weast 1984)
Molar Volume (cm³/mol):
145.2, 146.1 (20°C, 25°C, calculated-density)
162.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
32.037, 28.94 (25°C, at normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔHₙf (kJ/mol):
2.259 (at mp, Dreisbach 1959; Chickos et al. 1999)
2.36, 2.2 (–152.15, –25.45°C, Chickos et al. 1999)
Entropy of Fusion, ΔSₙf (J/mol K):
28.53, 36.7 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°C or as indicated and reported temperature dependence equations):
13840 (25.3°C, ebulliometry, measured range 12.6–81.8°C, Forziati et al. 1949)
log (P/mmHg) = 6.792930 – 1200.563/(226.650 + t°C); temp range 12.6–81.8°C (Antoine eq., ebulliometry-
manometer measurements, Forziati et al. 1949)
13650 (calculated from determined data, Dreisbach 1959)
log (P/mmHg) = 6.79230 – 1200.563/(226.050 + t°C); temp range 0 – 125°C (Antoine eq. for liquid state,
Dreisbach 1959)
13652 (derived from compiled data, temp range –18.8–205.94°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.79230 – 1200.563/(226.050 + t°C); temp range –18.8–205.94°C (Antoine eq., Zwolinski &
Wilhoit 1971)
13650, 13660 (interpolated-Antoine equations, Boublík et al. 1984)
log (P/kPa) = 5.92699 – 11206.087/(226.731 + t°C); temp range 22.7–105.6°C (Antoine eq. from reported exptl.
data, Boublík et al. 1984)
log (P/kPa) = 5.92037 – 1200.337/(226.256 + t°C); temp range 12.6–81.77°C (Antoine eq. from reported exptl.
data of Forziati et al. 1949, Boublík et al. 1984)
13650 (interpolated-Antoine eq., temp range –19 to 106°C, Dean 1985, 1992)
log (P/mmHg) = 6.79230 – 1200.563/(226.050 + t°C); temp range –19 to 106°C (Antoine eq., Dean 1985, 1992)
13650 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.9181 – 1201.098/(−47.026 + T/K); temp range 284–355 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.18145 – 1390.726/(−20.97 + T/K); temp range 353–483 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 32.3633 – 2.6614 × 10³/(T/K) – 8.7743·log (T/K) – 7.687 × 10⁻¹⁰·(T/K)²; temp range 249–531 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

241010 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{½}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH} (exptl) = 3.84 × 10¹² cm³ mol⁻¹ s⁻¹, k_{OH} (correlated) = 3.15 × 10¹² cm³ mol⁻¹ s⁻¹ at 296 K, measured range 296–498 K (flash photolysis-kinetic spectroscopy, Greiner 1970)

k_{OH} = (3.6 - 5.05) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296–305 K (Darnall et al. 1978)

k_{OH} = (4.21 ± 0.08) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = 5.23 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K, k_{OH} = 4.09 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 297 K (Atkinson 1985)

k_{OH}* = 4.23 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990)

k_{NO3} (exptl) = 2.23 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹, k_{NO3} (calc) = 1.31 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH}* = 4.24 × 10⁻¹² cm³ molecule⁻¹ s⁻¹, k_{NO3}* = 2.4 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:
2.1.1.1.8  n-Pentane

Common Name: n-Pentane
Synonym: pentane
Chemical Name: n-pentane
CAS Registry No: 109-66-0
Molecular Formula: C5H12; CH3(CH2)3CH3
Molecular Weight: 72.149
Melting Point (°C):
  –129.67  (Lide 2003)
Boiling Point (°C):
  36.06  (Lide 2003)
Density (g/cm³ at 20°C):
  0.6262, 0.6214  (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
  115.22, 116.1  (20°C, 25°C, calculated-density)
  118.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
  26.42, 25.77  (25°C bp, Dreisbach 1959)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
  8.393  (Dreisbach 1959; Riddick et al. 1986)
  8.4  (Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
  58.59, 63.2  (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
360  (16°C, cloud point, Fühner 1924)
120  (radiotracer method, Black et al. 1948)
38.5  (shake flask-GC, McAuliffe 1963, 1966)
49.7  (vapor saturation-GC, Barone et al. 1966)
40.0  (Baker 1967)
40.3*  (shake flask-GC, measured range 4 – 30°C, Nelson & De Ligny 1968)
11.8*  (shake flask-GC, measured range 5 – 35°C, Pierotti & Liabastre 1972)
65.7; 47.6, 44.6  (0, 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
39.5*  (shake flask-GC, measured range 25 – 149.5°C, Price 1976)
39.0  (shake flask-GC, Kryzanowska & Szeliwa 1978)
40.0  (partition coefficient, Rudakov & Lutsyk 1979)
40.75  (generator column-GC, Tewari et al. 1982a)
36.9  (calculated-activity coeff. γ and KOW, Tewari 1982b)
40.6*  (vapor saturation-GC, measured range 15 – 40°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°C, Shaw 1989)

\[
\ln x = -333.59719 + 14358.472/(T/K) + 47.97436\ln (T/K); \text{ temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)}
\]
44.09*  (calculated-liquid-liquid equilibrium LLE data, temp range 273.2 – 422.7 K, Mączyński et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

68213* (24.828°C, static method, measured range –65 to 25°C, Messerly & Kennedy 1940)

\[
\log (P/mmHg) = 6.87372 - \frac{1075.816}{233.369 + t/°C}; \text{ temp range 13.282–36.818°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)}
\]

71050* (interpolated-Antoine eq. regression, temp range –76.6 to 36.1°C, Stull 1947)
68330 (calculated from determined data, Dreisbach 1959)

\[
\log (P/mmHg) = 6.85221 - \frac{1064.63}{232.0 + t/°C}; \text{ temp range –35 to 80°C (Antoine eq. for liquid state, Dreisbach 1959)}
\]

68368* (interpolated-Antoine eq., temp range –50.14 to 57.53°C, Zwolinski & Wilhoit 1971)

\[
\log (P/mmHg) = 6.87632 - \frac{1075.78}{233.205 + t/°C}; \text{ temp range –50.14 to 57.53°C (Antoine eq., Zwolinski & Wilhoit 1971)}
\]

\[
\log (P/mmHg) = \left(-0.2185 \times \frac{6595.1}{T/K}\right) + 7.489673; \text{ temp range –76.6 to 191°C (Antoine eq., Weast 1972–73)}
\]

3400* (–30.86°C, gas saturation, measured range –129.54 to –30.86°C, Carruth & Kobayashi 1973)

57820* (20.57°C, ebulliometric method, measured range –4.4 to 68.218°C, Osborn & Douslin 1974)

68330 (interpolated-Antoine eq., Boublik et al. 1984)

\[
\log (P/kPa) = 6.12545 - \frac{1132.518}{239.074 + t/°C}; \text{ temp range –65.2 to 24.83°C (Antoine eq. from reported exptl data, Boublik et al. 1984)}
\]

\[
\log (P/kPa) = 5.96982 - \frac{1060.916}{231.577 + t/°C}; \text{ temp range 13.28–36.82°C (Antoine eq. from reported exptl data of Willingham et al. 1945, Boublik et al. 1984)}
\]

\[
\log (P/kPa) = 5.99028 - \frac{1071.187}{232.766 + t/°C}; \text{ temp range –4.4 to 68.21°C (Antoine eq. from reported exptl data of Osborn & Douslin 1974, Boublik et al. 1984)}
\]

70915 (interpolated-Antoine eq., temp range –50 to 58°C, Dean 1985, 1992)

\[
\log (P/mmHg) = 6.85296 - \frac{1064.021}{233.011 + t/°C}; \text{ temp range –50 to 58°C (Antoine eq., Dean 1985, 1992)}
\]

68330 (lit. average, Riddick et al. 1986)

\[
\log (P/kPa) = 5.97786 - \frac{1064.84}{232.012 + t/°C}; \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

68355 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/kPa) = 7.6922 - \frac{1686.65}{T/K}; \text{ temp range 143–233 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P/kPa) = 5.99466 - \frac{1073.139}{(–40.188 + T/K)}; \text{ temp range 223–352 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P/L/kPa) = 6.28417 - \frac{1260.973}{(–14.031 + T/K)}; \text{ temp range 350–422 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
\log (P/L/kPa) = 7.47436 - \frac{2414.137}{141.919 + T/K}; \text{ temp range 418–470 K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]

68340* (recommended, Ruzicka & Majer 1994)

\[
\ln \left[ \frac{(P/kPa)}{(P_o/kPa)} \right] = \left[ 1 - \frac{T_o/K}{T/K} \right] \cdot \exp \{2.73425 - 1.988544 \times 10^{-3} \cdot (T/K) + 2.408406 \times 10^{-6} \cdot (T/K)^2 \}; \text{ reference state at } P_o = 101.325 \text{ kPa, } T_o = 309.209 \text{ K (Cox equation, Ruzicka & Majer 1994)}
\]

\[
\log (P/mmHg) = 33.3239 - 2.4227 \times 10^9/(T/K) - 9.2354 \cdot \log (T/K) + 9.0199 \times 10^{-11} \cdot (T/K) + 4.105 \times 10^{-6} \cdot (T/K)^2; \text{ temp range 143–470 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

127050 (calculated as I/KAW, Cw/Ca, 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 (14.8, 20.05, 25.1, 30.1, 34.92°C, equilibrium cell-concentration ratio-GC, Jönsson et al. 1982)
121410* (calculated-temp dependence eq. derived from exptl data, measured range 15–35°C. Jönsson et al. 1982)
\[
\ln \left( \frac{1}{K_{\text{AW}}} \right) = \frac{19237.8}{(T/K)} + 53.671 \ln (T/K) - 372.214; \text{ temp range: } 15 - 35^\circ C \text{ (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)}
\]

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, \(\log K_{\text{OW}}\):**

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-\(k^\prime\) 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, \(\log K_{\text{OA}}\) at 25°C or as indicated:**

2.05*  (20.29°C, from GC-determined \(\gamma^\infty\) in octanol, measured range 20.29 – 50.28°C, Gruber et al. 1997)
1.95  (calculated-measured \(\gamma^\infty\) in pure octanol and vapor pressure \(P\), Abraham et al. 2001)

**Bioconcentration Factor, \(\log BCF\):**

**Sorption Partition Coefficient, \(\log K_{\text{OC}}\):**

**Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_\frac{1}{2}\):**

**Volatilization:**

**Photolysis:**

**Oxidation:**  rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{OH}}\) for reaction with \(OH\) radical, \(k_{\text{NO}_3}\) with \(NO_3\) radical and \(k_{\text{OS}}\) with \(O_3\) or as indicated *data at other temperatures see reference:

\(k_{\text{OS}} = 5.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) for the reaction with \(O(3P)\) (Herron & Huie 1973)

\(k_{\text{OH}} = (3.74 \pm 0.13) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 300 K (relative rate method, Darnall et al. 1978)

\(k_{\text{OH}} = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) (Atkinson et al. 1979)

\(k_{\text{OH}} = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{\text{OS}} = 5.8 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) room temp. (abstraction mechanism, Gaffney & Levine 1979)

\(k_{\text{OH}} = 4.13 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 299 ± 2 K (relative rate method, Atkinson et al. 1982a)

\(k_{\text{NO}_3} = (8.1 \pm 1.7) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296 K (relative rate method, Atkinson et al. 1984a; Atkinson 1991)

\(k_{\text{OH}} = (4.13 \pm 0.08) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at room temp. (relative rate, Atkinson et al. 1984c)

\(k_{\text{OH}} = 4.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 297 K (Atkinson 1986; quoted, Edney et al. 1986)

\(k_{\text{OH}} = 4.29 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 312 K in Smog chamber (Nolting et al. 1988)

\(k_{\text{OH}} = 3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (recommended, Atkinson 1989, 1991)

\(k_{\text{OH}} = 4.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{\text{NO}_3} = 8.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) (Sabljic & Güsten 1990)

\(k_{\text{NO}_3} = 8.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{\text{OH}} = 3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K with summer daylight atmospheric lifetime \(\tau = 35\) h (Altshuller 1991)

\(k_{\text{OH}} = 3.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K, \(k_{\text{NO}_3} = 9.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296 K (Atkinson 1990)

\(k_{\text{NO}_3}(\text{exptl}) = 8.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{\text{NO}_3}(\text{calc}) = 7.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)

\(k_{\text{OH}} = 4.00 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{\text{NO}_3} = 8.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (recommended, Atkinson 1997)

\(k_{\text{OH}} = 3.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

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Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

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

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<tr>
<th>TABLE 2.1.1.8.1</th>
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FIGURE 2.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for n-pentane.

TABLE 2.1.1.8.2
Reported vapor pressures of n-pentane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - B/(T/K) \quad (1)
\]

\[
\ln P = A - B/(T/K) \quad (1a)
\]

\[
\log P = A - B/(C + t/\degree C) \quad (2)
\]

\[
\ln P = A - B/(C + t/\degree C) \quad (2a)
\]

\[
\log P = A - B/(C + T/K) \quad (3)
\]

\[
\log \left( \frac{P/P_\Phi}{P_\Phi} \right) = A[1 - \Phi/(T/K)] \quad (5)
\]

\[
\ln \left[ \frac{(P/P_\Phi)/(P_\Phi/kPa)}{[(T_\Phi/K)/(T/K)]} \right] = \left[ 1 - (T_\Phi/K)/(T/K) \right] \exp\{A_0 - A_1(T/K) + A_2(T/K)^2\} \quad (6)
\]

where \( \log A = a + b(T/K) + c(T/K)^2 \) - Cox eq. I

- Cox eq. II

1. Messerly & Kennedy 1940
2. Willingham et al. 1945
3. Stull 1947
4. Zwolinski & Wilhoit 1971

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TABLE 2.1.1.8.2 (Continued)

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Carruth & Kobayashi 1973

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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

\[
\ln K_{AW} = A - \frac{B}{(T/K)} \quad (1) \\
\ln (1/K_{AW}) = A - \frac{B}{(T/K)} \quad (2) \\
\ln (k_f/\text{atm}) = A - \frac{B}{(T/K)} \quad (3) \\
\ln [H/(\text{Pa m}^3/\text{mol})] = A - \frac{B}{(T/K)} \quad (4) \\
K_{AW} = A - B(T/K) + C(T/K)^2 \quad (5)
\]

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<th>log ( K_{OA} )</th>
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<td><strong>Jönsson et al. 1982</strong></td>
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# interpolated from exptl data
FIGURE 2.1.1.8.3 Logarithm of Henry's law constant versus reciprocal temperature for \( n \)-pentane.

FIGURE 2.1.1.8.4 Logarithm of \( K_{OA} \) 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: C₆H₁₄; CH₃CH(CH₃)CH₂CH₂CH₃
Molecular Weight: 86.175
Melting Point (°C):
   –153.6 (Lide 2003)
Boiling Point (°C):
   60.26 (Lide 2003)
Density (g/cm³ at 20°C):
   0.6322, 0.6485 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
   136.31, 132.88 (20°C, 25°C, calculated-density)
   140.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
   29.87, 27.79 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
   6.203 (Dreisbach 1959)
   6.268 (Riddick et al. 1986)
   6.27 (Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
   52.43, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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  (0, 25°C, 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°C, Price 1976)
   13.7* (recommended best value, temp range 25 – 150°C, IUPAC Solubility Data Series, Shaw 1989a)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
   29040* (25.64°C, ebulliometry, measured temp range 12.758–61.066°C, Willingham et al. 1945)
   log (P/mmHg) = 6.83910 – 1135.410/(226.572 + t°C); temp range 12.758–61.066°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
   27820* (calculated-Antoine eq. regression, temp range –60 to 60.3°C, Stull 1947)
   28200* (calculated from determined data, Dreisbach 1959)
   log (P/mmHg) = 6.83910 – 1135.410/(226.572 + t°C); temp range –15 to 100°C (Antoine eq. for liquid state, Dreisbach 1959)
   28238; 28200* (derived from compiled, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.83910 – 1135.410/(226.572 + t°C); temp range –32.1 to 83.4°C (Antoine eq., Zwolinski & Wilhoit 1971)
   27780 (interpolated-Antoine eq., Weast 1972-73)
log \( (P/\text{mmHg}) = [-0.2185 \times 7676.6/(T/\text{K})] + 7.944630 \); temp range: -60.9 to 60.3°C (Antoine eq., Weast 1972–73)

28240 (interpolated-Antoine eq., Boublik et al. 1984)

log \( (P/\text{kPa}) = 6.86839 - 1151.401/(228.476 + t/\text{°C}) \); temp range 12.78 – 61°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°C, Dean 1985, 1992)

log \( (P/\text{mmHg}) = 6.83910 - 1135.41/(226.570 + t/\text{°C}) \); temp range -32 to 83°C (Antoine eq., Dean 1985, 1992)

28300 (selected lit., Riddick et al. 1986)

log \( (P/\text{mmHg}) = 6.83910 - 1135.41/(226.570 + t/\text{°C}) \); temp range -32 to 83°C (Antoine eq., Dean 1985, 1992)

28250 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log \( (P/\text{mmHg}) = 30.7477 - 2.4888 \times 10^3/(T/\text{K}) -8.2295 \cdot \log (T/\text{K}) - 2.3723 \times 10^{-11} \cdot (T/\text{K})^2 \); temp range 120–498 K (vapor pressure eq., Yaws 1994)

72190 (50°C, vapor-liquid equilibria VLE data, Horstmann et al. 2004)

log \( (P/\text{kPa}) = 5.99313 - 1151.40/(T/\text{K} - 44.673) \); temp range not specified (Antoine eq., Horstmann et al. 2004)

Henry’s Law Constant (Pa m^3/mol at 25°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/K_{AW}, C_{AW}/C_{X}, 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°C, Ashworth et al. 1988)

\[ \ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = 2.959 - 957.2/(T/\text{K}) \] \( \text{temp range} 10 \text{–} 30^\circ \text{C} \) (EPICS measurements, Ashworth et al. 1988)

76280 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

746 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log \( K_{AW} = 2.470 - 288/(T/\text{K}) \) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

2.80 (calculated-π constant, Hansch et al. 1968)

2.85 (calculated-MCI \( \chi \), Murray et al. 1975)

3.23 (calculated-molar volume \( V_m \), Wang et al. 1992)

3.74 (calculated-fragment constant, Müller & Klein 1992)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_3 radical and \( k_{O3} \) with O_3 or as indicated, *data at other temperatures see reference:

\[ k_{OH}(\text{exptl}) = (3.2 \pm 0.6) \times 10^9 \text{M}^{-1} \text{s}^{-1} \text{ at} 305 \pm 2 \text{K} \] (relative rate method, Lloyd et al. 1976, Darnall et al. 1976)

\[ k_{OH} = (5.68 \pm 0.24) \times 10^{12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at} \text{ room temp.} \] (relative rate, Atkinson et al. 1984c)

\[ k_{OH} = 5.6 \times 10^{12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at} 298 \text{K} \] (recommended, Atkinson 1989, 1990)

\[ k_{OH} = 2.34 \times 10^{12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at} 298 \text{K} \] (recommended, Atkinson 1990)

\[ k_{OH} = 5.6 \times 10^{12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}, \text{ estimated atmospheric lifetime was} 25 \text{h during summer daylight hours} \] (Altshuller 1991)

\[ k_{NO3}(\text{exptl}) = 1.71 \times 10^{-16} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}, k_{NO3}(\text{calc}) = 1.83 \times 10^{-16} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at} 296 \pm 2 \text{K} \] (relative rate method, Aschmann & Atkinson 1995)

\[ k_{OH} = 5.3 \times 10^{-12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}, k_{NO3} = 1.8 \times 10^{-16} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at} 298 \text{K} \] (recommended, Atkinson 1997)
Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: half-life of 2.4–24 h based on photooxidation rate constant of $3.2 \times 10^{12}$ cm³ mol⁻¹ 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 $5.6 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ for the reaction with hydroxyl radical in air (Altshuller 1991).

### TABLE 2.1.1.9.1

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<tr>
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<td>shake flask-GC</td>
<td>IUPAC recommended</td>
<td>calc-recommended LLE data</td>
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<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
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**FIGURE 2.1.1.9.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methylpentane.
TABLE 2.1.1.9.2
Reported vapor pressures and Henry’s law constants of 2-methylpentane at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
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<tr>
<td><strong>ebulliometry</strong></td>
<td><strong>summary of literature data</strong></td>
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<td>t/°C</td>
<td>P/Pa</td>
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<td>16620</td>
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<td>16.82</td>
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<td>20.584</td>
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<td>25.617</td>
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<td>30.237</td>
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<td>B</td>
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<td>C</td>
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</tr>
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</table>

\[ \log P = A - \frac{B}{T(K)} \]  
\( (1) \)

\[ \log P = A - \frac{B}{(C + t/°C)} \]  
\( (2) \)

\[ \log P = A - \frac{B}{(C + T/K)} \]  
\( (3) \)

\[ \log P = A - \frac{B}{T(K)} - C \cdot \log (T/K) \]  
\( (4) \)

\[ \ln \left( \frac{P}{P_{ref}} \right) = \left[ 1 - \left( \frac{T_{ref}}{T} \right) \right] \cdot \exp\left( a + bT + cT^2 \right) \]  
\( (5) \)

\[ \ln H = A - \frac{B}{T(K)} \]

\[ H/(\text{atm m}^3/\text{mol}) \]

\[ \Delta H_f/(kJ \text{ mol}^{-1}) = \]

at 25°C 29.76

at bp 27.79

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FIGURE 2.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpentane.

FIGURE 2.1.1.9.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-methylpentane.
3-Methylpentane

Common Name: 3-Methylpentane
Synonym: diethylmethylmethane
Chemical Name: 3-methylpentane
CAS Registry No: 96-14-0
Molecular Formula: C₆H₁₄; CH₃CH₂(CH₃)CHCH₂CH₃
Molecular Weight: 86.175
Melting Point (°C):
-162.9 (Lide 2003)
Boiling Point (°C):
63.27 (Lide 2003)
Density (g/cm³ at 25°C):
0.66431, 0.65976 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
129.7, 130.6 (20°C, 25°C, calculated-density)
190.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
30.28, 28.08 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
5.035 (Riddick et al. 1986)
5.31 (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
48.17, 50.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
12.8 (shake flask-GC, McAuliffe 1966)
21.5; 17.9, 17.2 (0; 25°C, 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 (0, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
29040 (23.2°C, ebulliometry, measured range 15.29–64.083°C, Willingham et al. 1945)
\[ \log (P/\text{mmHg}) = 6.84887 - 1152.368/(227.129 + t/°C); \text{ temp range 15.29–64.083°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)} \]
24970 (Antoine eq. regression, temp range –59 to 63.3°C, Stull 1947)
25300 (calculated from determined data, Dreisbach 1959)
\[ \log (P/\text{mmHg}) = 6.84887 - 1152.368/(227.129 + t/°C); \text{ temp range –15 to 105°C (Antoine eq. for liquid state, Dreisbach 1959)} \]
25305, 25300 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 6.84887 - 1152.368/(227.129 + t/°C); \text{ temp range –30.1 to 86.6°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]
24940 (interpolated-Antoine eq., Weast 1972–73)
\[ \log (P/\text{mmHg}) = [-0.2185 \times 7743.9/(T/K)] + 7.947042; \text{ temp range –59 to 63.3°C (Antoine eq., Weast 1972–73)} \]
25310 (interpolated-Antoine eq, Boublik et al. 1984)
log (P/kPa) = 6.36895 – 1997.558/(202.608 + t°C); temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

25300 (interpolated-Antoine eq., temp range –30 to 87°C, Dean 1985, 1992)
log (P/mmHg) = 6.84887 – 1152.368/(227.13 + t°C); temp range –30 to 87°C (Antoine eq., Dean 1985, 1992)

25300 (lit. average, Riddick et al. 1986)
log (P/kPa) = 5.98356 – 11133.52/(224.944 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

25320 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.97897 – 1155.28/(–45.659 + T/K); temp range 293–338 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 35.2848 – 2.6773 × 10^3/(T/K) – 9.8546·log (T/K) + 2.2352 × 10^–11·(T/K)^2; temp range 110–504 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
172000 (recommended; Mackay & Shiu 1981)
171490 (calculated as 1/K_{AW} C_w/C_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 K_{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 \nu_i and solvatochromic parameters, Leahy 1986)
3.60 ± 0.20 (recommended, Sangster 1989)
3.18 (calculated-molar volume \nu_M, Wang et al. 1992)
3.74 (calculated-fragment constant, Mülher & Klein 1992)
2.9168 (calculated-UNIFAC group contribution, Chen et al. 1993)
3.60 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_0:

Volatileization:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3, or as indicated, *data at other temperatures see reference:

k_{OH} = 1.28 \times 10^9 L mol^{-1} s^{-1} at 300 K (Greiner 1967; quoted, Altshuller & Bufalini 1971)

k_{OH} = (4.3 \pm 0.9) \times 10^8 M^{-1} s^{-1} at 305 \pm 2 K (relative rate method, Lloyd et al. 1976)

k_{OH} = 6.82 \times 10^{-12} cm^3 molecule^{-1} s^{-1} at atmospheric pressure and 305 K (Darnall et al. 1978)

k_{OH} = (5.78 \pm 0.11) \times 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (relative rate, Atkinson et al. 1984c)

k_{OH} = 5.7 \times 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989, 1990, 1991)

k_{OH} = 5.7 \times 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K, estimated atmospheric lifetime 25 h, during summer daylight hours (Altshuller 1991)

k_{NO_3}(exptl) = 2.04 \times 10^{-16} cm^3 molecule^{-1} s^{-1}, k_{NO_3}(calc) = 2.53 \times 10^{-16} cm^3 molecule^{-1} s^{-1} at 296 \pm 2 K (relative rate method, Aschmann & Atkinson 1995)

k_{OH} = 5.4 \times 10^{-12} cm^3 molecule^{-1} s^{-1}, k_{NO_3} = 2.2 \times 10^{-16} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: photooxidation reaction rate constant of $4.30 \times 10^{12}$ cm$^3$ mol$^{-1}$ s$^{-1}$ with hydroxyl radical with half-life of 2.4–24 h (Darnall et al. 1976; Lloyd et al. 1976);
rate constant of $5.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$·s$^{-1}$ for the reaction with OH radical with an estimated atmospheric lifetime of 25 h during summer daylight (Altshuller 1991).
Common Name: 2,2-Dimethylpentane  
Synonym:  
Chemical Name: 2,2-dimethylpentane  
CAS Registry No: 590-35-2  
Molecular Formula: C₇H₁₆; CH₃C(CH₃)₂CH₂CH₂CH₃  
Molecular Weight: 100.202  
Melting Point (°C):  
-123.7 (Lide 2003)  
Boiling Point (°C):  
79.2 (Lide 2003)  
Density (g/cm³ at 20°C):  
0.6739 (Weast 1984)  
0.6739, 0.6695 (20°C, 25°C, Dreisbach 1959)  
Molar Volume (cm³/mol):  
148.69 (20°C, calculated from density)  
162.8 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ∆H_fus (kJ/mol):  
5.812 (Dreisbach 1959)  
5.86 (Chickos et al. 1999)  
Entropy of Fusion, ∆S_fus (J/mol K):  
39.55, 49.74 (exptl., calculated-group additivity method, Chickos et al. 1999)  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
4.40 (shake flask-GC, Price 1976)  
4.90 (calculated-recommended liquid-liquid equilibrium LLE data, Maczyński et al. 2004)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):  
13824 (24.67°C, manometer, measured range 15.325–80.05°C, Willingham et al. 1945)  
log (P/mmHg) = 6.81509 – 1190.298/(223.343 + t/°C); temp range 15.325–80.05°C (Antoine eq. from exptl. data, ebulliometry-manometer measurements, Willingham et al. 1945)  
13850 (24.708°C, ebulliometry, Forzìati et al. 1949)  
log (P/mmHg) = 6.81479 – 1190.033/(223.303 + t/°C); temp range 12.188–80.074°C (Antoine eq., ebulliometry-manometer measurements, Forzìati et al. 1949)  
14030 (calculated from determined data, Dreisbach 1959)  
log (P/mmHg) = 6.81480 – 1190.033/(223.303 + t/°C); temp range 0–115°C (Antoine eq. for liquid state, Dreisbach 1959)  
14026 (interpolated-Antoine eq., temp range –18.6 to 103.75°C, Zwolinski & Wilhoit 1971)  
log (P/mmHg) = 6.81480 – 1190.033/(223.303 + t/°C); temp range –18.6 to 103.75°C (Antoine eq., Zwolinski & Wilhoit 1971)  
13500 (interpolated-Antoine eq., temp range –69.3 to 49.7°C, Weast 1972–73)  
log (P/mmHg) = [-0.2185 × 7271.0/(T/K)] + 7.841340; temp range –69.3 to 49.7°C (Antoine eq., Weast 1972–73)  
14030 (interpolated-Antoine eq., Boublík et al. 1984)  
log (P/kPa) = 5.93788 – 1189.09/(223.198 + t°C); temp range 15.32-80.05°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublík et al. 1984)  
14030 (interpolated-Antoine eq., temp range –18 to 103°C, Dean 1985, 1992)  
log (P/mmHg) = 6.81480 – 1190.033/(223.3 + t°C); temp range –18 to 103°C (Antoine eq., Dean 1985, 1992)  
14010 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log \((P_{L}/kPa) = 5.93117 – 1185.576/(–50.37 + T/K)\); temp range 277-354 K (Antoine eq.-I, Stephenson & Malanowski 1987)


log \((P/mmHg) = 6.2875 – 2.1682 \times 10^3/(T/K) + 2.6936 \cdot \log (T/K) – 1.5525 \times 10^{-2} \cdot (T/K) + 1.0917 \times 10^{-5} \cdot (T/K)^2\); temp range 149–527 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°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 \(K_{OW}\):

3.10  (calculated-π substituent constant, Hansch et al. 1968)
3.62  (calculated-V_{M}, Wang et al. 1992)
4.14  (calculated-fragment constant, Müller & Klein 1992)

Octanol/Air Partition Coefficient, log \(K_{OA}\):

Bioconcentration Factor, log \(BCF\):

Sorption Partition Coefficient, log \(K_{OC}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_\text{½}\):

Volatilization:

Photolysis:

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with NO₃ radical and \(k_{O3}\) with O₃ or as indicated, *data at other temperatures see reference:

\[
k_{OH} = 2.66 \pm 0.08 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (relative rate, Atkinson et al. 1984c)}
\]

\[
k_{OH} = 3.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K (Atkinson 1989)}
\]

\[
k_{OH} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1990)}
\]

\[
k_{OH} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, } k_{NO3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (Atkinson 1990)}
\]

\[
k_{OH} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\(k_1\)) and Elimination (\(k_2\)) Rate Constants or Half-Lives:

Half-Lives in the Environment:
2.1.1.12 2,4-Dimethylpentane

Common Name: 2,4-Dimethylpentane
Synonym: diisopropylmethane
Chemical Name: 2,4-dimethylpentane
CAS Registry No: 108-08-7
Molecular Formula: \( \text{C}_7\text{H}_{16} \)
Molecular Weight: 100.202
Melting Point (°C):
-119.5 (Lide 2003)
Boiling Point (°C):
80.49 (Lide 2003)
Density (g/cm\(^3\) at 20°C):
- 0.6727, 0.6683 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm\(^3\)/mol):
- 148.95, 149.9 (20°C, 25°C, calculated-density)
- 162.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
- 6.840 (Dreisbach 1959)
- 6.845 (Riddick et al. 1986)
- 6.85 (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
- 44.46, 44.7 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°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 (0; 25°C, 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 (0, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
- 12635 (Antoine eq. regression, temp range –48 to 80.5°C, Stull 1947)
- \( \log (P/\text{mmHg}) = 6.82621 - 1192.041/(221.634 + t/°C) \); temp range 13.714 – 81.374°C (Antoine eq. from exptl. data, ebulliometry-manometer, Forziati et al. 1949)
- 13120 (calculated from determined data, Dreisbach 1959)
- \( \log (P/\text{mmHg}) = 6.82621 - 1192.041/(221.634 + t/°C) \); temp range 0 – 115°C (Antoine eq. for liquid state, Dreisbach 1959)
- 13119 (interpolated-Antoine eq, temp range –17.0 to 104.94°C, Zwolinski & Wilhoit 1971)
- \( \log (P/\text{mmHg}) = 6.82621 - 1192.041/(221.634 + t/°C) \); temp range –17.0 to 104.94°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 12620 (interpolated-Antoine eq., temp range –48.0 to 80.5°C, Weast 1972–73)
- \( \log (P/\text{mmHg}) = [-0.2185 \times 8167.4/(T/K)] + 7.961374 \); temp range –48.0 to 80.5°C (Antoine eq., Weast 1972–73)
- \( \log (P/\text{mmHg}) = 5.95675 - 1195.154/(221.992 + t/°C) \); temp range 13.7 – 81.37°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
15450  (interpolated-Antoine eq., temp range –17 to 105°C, Dean 1985, 1992)
log \( (P/\text{mmHg}) = 6.82621 - 1192.04/(225.32 + t/°C) \); temp range –17 to 105°C (Antoine eq., Dean 1985, 1992)
13000  (selected, Riddick et al. 1986)
log \( (P/\text{kPa}) = 5.94917 - 1191.06/(221.540 + t/°C) \); temp range not specified (Antoine eq., Riddick et al. 1986)
13125  (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log \( (P/\text{kPa}) = 5.95921 - 1196.516/(-50.993 + T/K) \); temp range 284–355 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
319300  (calculated–1/KAW, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
326600, 73120  (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
300000  (recommended; Mackay & Shiu 1981)
297300  (calculated-P/C, Eastcott et al. 1988)
160050  (calculated-molecular connectivity index MCI χ, Nirmalakhandan & Speece 1988)
298050  (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \( K_{OW} \):
3.10  (calculated-π constant, Hansch et al. 1968)
3.17  (calculated-MCI χ, Murray et al. 1975)
3.66  (calculated-molar volume \( V_M \), Wang et al. 1992)
4.14  (calculated-f constant, Müller & Klein 1992)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):
Volatilization:
Photolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO3 radical and \( k_{O3} \) with O3 or as indicated, *data at other temperatures see reference:

Volatilization:
Photolysis:
Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO3 radical and \( k_{O3} \) with O3 or as indicated, *data at other temperatures see reference:

Air: photooxidation reaction rate constant of \( 5.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with hydroxyl radicals and an estimated lifetime of 27 h during summer daylight (Altshuller 1991).
2.1.1.1.13 3,3-Dimethylpentane

Common Name: 3,3-Dimethylpentane

Synonym:

Chemical Name: 3,3-dimethylpentane

CAS Registry No: 562-49-2

Molecular Formula: C\(_7\)H\(_{16}\); CH\(_3\)CH\(_2\)(CH\(_3\))\(_2\)CH\(_2\)CH\(_3\)

Molecular Weight: 100.202

Melting Point (°C):
- 134.4 (Lide 2003)

Boiling Point (°C):
- 86.06 (Lide 2003)

Density (g/cm\(^3\) at 20°C):
- 0.6933, 0.6891 (20°C, 25°C, Dreisbach 1959)

Molar Volume (cm\(^3\)/mol):
- 144.5 (20°C, calculated-density, Stephenson & Malanowski 1987)
- 162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
- 33.02, 29.74 (25°C, normal bp, Dreisbach 1959)

Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
- 7.067 (Dreisbach 1959)
- 7.07 (Chickos et al. 1999)

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

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°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°C, Price 1976)

Vapor Pressure (Pa at 25°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°C Stull 1947)
- 10316* (23.521°C, ebulliometry, measured range –13.5 to 82°C Forziati et al. 1949)
  \[
  \log (P/mmHg) = 6.82668 – 1228.063/(225.316 + t/°C); \text{ temp range 13.484–80.962°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)}
  \]
- 11044 (calculated from determined data, Dreisbach 1959)
  \[
  \log (P/mmHg) = 6.82667 – 1228.663/(225.316 + t/°C); \text{ temp range 5–130°C (Antoine eq. for liquid state, Dreisbach 1959)}
  \]
- 11039* (interpolated-Antoine eq., temp range –14.4 to 111.25°C, Zwolinski & Wilhoit 1971)
  \[
  \log (P/mmHg) = 6.8267 – 1228.663/(225.316 + t/°C); \text{ temp range –14.4 to 111.25°C (Antoine eq., Zwolinski & Wilhoit 1971)}
  \]
- 10600 (interpolated-Antoine eq., temp range –45.9 to 86.1°C, Weast 1972–73)
  \[
  \log (P/mmHg) = [–0.2185 \times 8145.4/(T/K)] + 7.869254; \text{ temp range –45.9 to 86.1°C (Antoine eq., Weast 1972–73)}
  \]
- 11045 (interpolated-Antoine eq., temp range 13.484–86.96°C, Boublik et al. 1984)
  \[
  \log (P/kPa) = 5.95327 – 1229.625/(225.427 + t/°C); \text{ temp range 13.484–86.96°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
  \]
- 11045 (interpolated-Antoine eq., temp range –14 to 112°C, Dean 1985, 1992)
log (P/mmHg) = 6.82667 – 1228.663/(225.32 + t/°C); temp range –14 to 112°C (Antoine eq., Dean 1985, 1992)
11150, 11040 (interpolated-Antoine eq.-I, III, Stephenson & Malanowski 1987)
log (P/kPa) = 5.95139 – 1228.138/(–47.819 + T/K); temp range 285–360 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.35011 – 1415.316/(–31.302 + T/K); temp range 213–281 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/kPa) = 5.94685 – 1225.973/(–48.144 + T/K); temp range 280–360 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = 30.2570 – 2.6313×10³/(T/K) – 7.9839·log (T/K) + 4.6848 × 10⁻¹³·(T/K) + 2.717 × 10⁻⁶·(T/K)²; temp range 139–536 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
186000 (calculated-P/C, Mackay & Shiu 1981)
186305 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Air Partition Coefficient, log K_{OA}:
Octanol/Water Partition Coefficient, log K_{OW}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k and Half-Lives, t_{½}:

Half-Lives in the Environment:

<table>
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<tr>
<th>TABLE 2.1.1.13.1</th>
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<td>Reported aqueous solubilities of 3,3-dimethylpentane at various temperatures</td>
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<th>Price 1976</th>
<th>Maćzyński et al. 2004</th>
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<td>shake flask-GC</td>
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**FIGURE 2.1.1.13.1** Logarithm of mole fraction solubility \((\ln x)\) versus reciprocal temperature for 3,3-dimethylpentane.

**TABLE 2.1.1.13.2**

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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\ln P &= A - B/(C + T/K) \quad (3a) \\
\log P &= A - B/(T/K) - C\cdot\log (T/K) \quad (4) \\
\ln (P/P_{ref}) &= [1 - (Tref/T)]\cdot\exp(a + bT + cT^2) \quad (5)
\end{align*}
\]

**Stull 1947**

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<th>\text{P}^{/\text{Pa}}</th>
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**Forziati et al. 1949**

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**Zwolinski & Wilhoit 1971**

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<td>33.02</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>at bp</td>
<td>29.65</td>
<td></td>
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</tr>
</tbody>
</table>

**FIGURE 2.1.1.13.2** Logarithm of vapor pressure versus reciprocal temperature for 3,3-dimethylpentane.
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: C₈H₁₈; CH₃C(CH₃)₂CH₂CH(CH₃)CH₃
Molecular Weight: 114.229
Melting Point (°C):
—107.30 (Stull 1947; Lide 2003)
Boiling Point (°C):
99.22 (Lide 2003)
Density (g/cm³ at 20°C):
0.6919, 0.6878 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
165.1 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
185.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
36.92, 32.01 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
9.196 (Riddick et al. 1986)
9.27 (Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
55.52, 43.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
2.44 (shake flask-GC, McAuliffe 1963, 1966)
2.46; 2.05 (0; 25°C, shake flask-GC, Polak & Lu 1973)
1.14 (shake flask-GC, Price 1976)
2.50, 2.0, 2.20 (0, 20, 25°C, IUPAC recommended values, Shaw 1989b)
2.30, 1.65, 1.65 (0, 20, 25°C, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
6371 (24.4°C, ebulliometry, measured temp range 24.4–100.13°C, Willingham et al. 1945)
log (P/mmHg) = 6.81189 – 1257.840/(220.735 + t°C); temp range 24.4–100.13°C (Antoine eq., ebulliometry-manometer measurements, Willingham et al. 1945)
6250 (calculated-Antoine eq. regression, temp range –36.4 to 99°C, Stull 1947)
1739, 6573, 19528 (0, 25, 50°C, static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)
6580 (calculated from determined data, Dreisbach 1959; quoted, Hine & Mookerjee 1975)
log (P/mmHg) = 6.81189 – 1257.840/(220.735 + t°C); temp range 15 – 120°C (Antoine eq. for liquid state, Dreisbach 1959)
6573 (interpolated-Antoine eq., temp range –4.3 to 125.22°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.81189 – 1257.840/(220.735 + t°C); temp range –4.3 to 125.22°C (Antoine eq., Zwolinski & Wilhoit 1971)
6570 (interpolated-Antoine eq., temp range 24.6–100.13°C, Boublík et al. 1973, 1984)
log (P/mmHg) = 6.80304 – 1252.59/(220.119 + t°C), temp range 24.6–100.13°C (Antoine eq. from reported extpl. data of Willingham et al. 1945, Boublík et al. 1984)
6240 (interpolated-Antoine eq., temp range –36.5 to 99.2°C, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 8548.0/(T/K)] + 7.934852; temp range –36.5 to 99.2°C (Antoine eq., Weast 1972–73)
\[
\log (P/kPa) = 5.92751 - 1252.348/(220.09 + t/°C); \text{ temp range } 69.2 - 271.1°C \text{ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)}
\]
6580 (interpolated-Antoine eq., temp range: 24 – 100°C, Dean 1985, 1992)
\[
\log (P/mmHg) = 6.81189 - 1257.84/(220.74 + t/°C), \text{ temp range: 24 – 100°C (Antoine eq., Dean 1985, 1992)}
\]
6500 (quoted lit., Riddick et al. 1986)
\[
\log (P/kPa) = 5.92885 - 1153.36/(220.241 + t/°C), \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]
6580 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/kPa) = 5.93934 - 1254.146/(-52.831 + T/K), \text{ temp range: 297–314 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.44016 - 1650.17/(T/K); \text{ temp range 423–523 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.33252 - 1441.485/(-36.695 + T/K); \text{ temp range 194–299 K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]
\[
\log (P/kPa) = 6.97534 - 1283/067/(-40.166 + T/K); \text{ temp range 372–416 K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]
65200 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P/kPa) = 7.76427 - 3268.783/(206.659 + T/K); \text{ temp range 490–544 K (Antoine eq.-VI, Stephenson & Malanowski 1987)}
\]
\[
\log (P/mmHg) = 35.954 - 3.0569 \times 10^3/(T/K) - 9.8896 \times \log (T/K) - 7.2916 \times 10^{-11} \times (T/K) + 3.1060 \times 10^{-6} \times (T/K)^2; \text{ temp range 161–564 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C):
308030 (calculated-P/C, Mackay & Leinonen 1975)
330000; 308000, 365000 (recommended; calculated-P/C, Mackay & Shiu 1981)
304960 (calculated as 1/Kₖ₃, Cₖ₄/Cₖ₅, reported as exptl., Hine & Moorjeree 1975)
472090, 110700 (calculated-group contribution, calculated-bond contribution, Hine & Moorjeree 1975)
314110 (calculated-P/C, Lyman et al. 1982)
350140 (calculated-MCI χ, 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 Kₜₖₚ:
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 Vₚ, Wang et al. 1992)

Octanol/Air Partition Coefficient, log Kₜₖₚ:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log Kₜₖₚ:

Environmental Fate Rate Constants, k, and Half-Lives, tₜₖ:
Volatilization: volatilization tₜₖ = 5.5 h from a water column 1 m² in cross section of depth 1 m (Mackay & Leinonen 1975);
tₜₖ = 3.1 h at 20°C in a river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (estimated, Lyman et al. 1982).
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, kₖₚ for reaction with OH radical, kₖₚ with NO₃ radical and kₖₚ with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
kₖₚ*(exptl) = 2.83 \times 10^{12} \text{ cm}³ \text{ mol}⁻¹ \text{ s}⁻¹, kₖₚ(calc) = 2.35 \times 10^{12} \text{ cm}³ \text{ mole}⁻¹ \text{ s}⁻¹ at 298 K, measured range 298–493 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
kₖₚ = 3.73 \times 10^{12} \text{ cm}³ \text{ molecule}⁻¹ \text{ s}⁻¹ at room temp. (Darnall et al. 1978)
k_{O(3P)} = 9.10 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O(3P) atom at room temp. (Herron & Huie 1973)}

k_{OH} = 3.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson et al. 1979)}

k_{O_3}^{*} = 2.0 \times 10^{-23} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K, measured range 298–323 K (Atkinson & Carter 1984)}

k_{OH} = (3.66 \pm 0.16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (relative rate, Atkinson et al. 1984c)}

k_{OH} = 3.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K and 3.56 \times 10^{-12} cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 297 K (Atkinson 1985)}

k_{OH} = 3.68 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989, 1990)}

k_{NO_3}^{(exptl)} = 7.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3}^{(calc)} = 1.65 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 ± 2 K (relative rate method, Aschmann & Atkinson 1995)}

k_{OH}^{*} = 3.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 9.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1997)}

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (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} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} with OH radical in air during summer daylight (Altshuller 1991).

Surface water: volatilization t_\text{1/2} = 5.5 h from a water column 1 m^2 in cross section of depth 1-m (Mackay & Leinonen 1975);

estimated t_\text{1/2} = 3.1 h at 20°C in a river 1 m deep flowing at 1 m/s with a wind velocity of 3 m 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: C₈H₁₈; CH₃CH(CH₃)CH(CH₃)CH(CH₃)CH₃
Molecular Weight: 114.229
Melting Point (°C):
  –109.2 (Lide 2003)
Boiling Point (°C):
  113.5 (Lide 2003)
Density (g/cm³ at 20°C):
  0.7191 (Weast 1984)
  0.7191, 0.7191 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
  158.9 (calculated-density, Stephenson & Malanowski 1987)
  185.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  38.0, 32.67 (25°C, at normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔHfus (kJ/mol):
  9.27 (Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
  56.65, 38.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
  2.34, 2.30 (0; 25°C, 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°C, calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

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

Henry’s Law Constant (Pa m3/mol at 25°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 K_{ow}:

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volutilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
with NO3 radical and k_{O3} with O3, or as indicated, *data at other temperatures and/or the Arrhenius expression
see reference:
k_{OH} = 6.99 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 295 K, measured range 243–313 K (relative rate method with
reference to n-hexane, Harris & Kerr 1988; Atkinson 1989)
k_{OH} = 7.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1990)
k_{OH} = 7.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K and the atmospheric lifetime was estimated to be 20 h during
summer daylight hours (Altshuller 1991)
k_{OH} = 7.1 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) 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 × 10^{-12} cm³ molecule⁻¹ s⁻¹ with OH radicals in air during summer daylight (Altshuller 1991).
2.1.1.1.16 n-Hexane

<table>
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<tr>
<th>Property</th>
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</thead>
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<td>n-Hexane</td>
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<td>Synonym</td>
<td>hexane</td>
</tr>
<tr>
<td>Chemical Name</td>
<td>n-hexane</td>
</tr>
<tr>
<td>CAS Registry No</td>
<td>110-54-3</td>
</tr>
<tr>
<td>Molecular Formula</td>
<td>C₆H₁₄; CH₃(CH₂)₄CH₃</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>86.175</td>
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<td>Melting Point (°C)</td>
<td>–95.35 (Lide 2003)</td>
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<td>Boiling Point (°C)</td>
<td>68.73 (Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C)</td>
<td>0.6593, 0.6548 (20°C, 25°C, Riddick et al. 1986)</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol)</td>
<td>130.7; 131.6 (20°C, 25°C, calculated-density)</td>
</tr>
<tr>
<td>Enthalpy of Vaporization, ΔHᵥ (kJ/mol)</td>
<td>31.552, 28.853 (25°C, bp, Riddick et al. 1986)</td>
</tr>
<tr>
<td>Entropy of Fusion, ΔSᵥ (J/mol K)</td>
<td>73.22, 72.5 (exptl., calculated-group additivity method, Chickos et al. 1999)</td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.)</td>
<td>140 (15.5°C, shake flask-cloud point, Fühner 1924)</td>
</tr>
</tbody>
</table>

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
Aliphatic and Cyclic Hydrocarbons

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

24811* (30°C, static-manometer, measured range 30–60°C, Smyth & Engel 1929)
19920* (24.7°C, ebulliometry, measured range 13.03–69.54°C Willingham et al. 1945)

\[ \log (P/\text{mmHg}) = 6.87776 – 1171.530/(224.366 + t/°C); \text{ temp range 13.03–69.54°C} \] (Antoine eq. from exptl. data, ebulliometry, Willingham et al. 1945)
19700* (calculated-Antoine eq. regression, temp range –53.9 to 68.7°C, Stull 1947)
20170 (calculated from determined data, Dreisbach 1959)

\[ \log (P/\text{mmHg}) = 6.87776 – 1171.53/(224.366 + t/°C); \text{ temp range –10 to 110°C} \] (Antoine eq. for liquid state, Dreisbach 1959)
20198* (interpolated-Antoine eq., temp range –25.1 to 92.1°C, Zwolinski & Wilhoit 1971)

20130 (Campbell et al. 1968)
20124, 20141 (static method-differential pressure gauge, Bissell & Williamson 1975)
22090* (27.1°C, Letcher & Marsicano 1974)
20160 (interpolated-Antoine eq., Boublik et al. 1984)

\[ \log (P/\text{kPa}) = 6.01098 – 1176.102/(224.899 + t/°C); \text{ temp range 13.03–69.54°C} \] (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
20190 (interpolated-Antoine eq., temp range –25 to 92°C, Dean 1985, 1992)

\[ \log (P/\text{kPa}) = 5.72763 – 1031.938/(208.304 + t/°C); \text{ temp range 27.11–45.11°C} \] (Antoine eq. from reported exptl. data of Letcher & Marsicano 1974, Boublik et al. 1984)

20190 (interpolated-Antoine eq., temp range –25 to 92°C, Dean 1985, 1992)

\[ \log (P/\text{kPa}) = 6.00091 – 1171.91/(224.408 + t/°C), \text{ temp range not specified} \] (Antoine eq., Riddick et al. 1986)
20180, 20300, 20165 (interpolated-Antoine equations I, II and IV , Stephenson & Malanowski 1987)

\[ \log (P\text{L}/\text{kPa}) = 6.4106 – 1469.286/(–7.702 + T/K); \text{ temp range 374–451 K} \] (Antoine eq.-VI, Stephenson & Malanowski 1987)
\[ \log (P\text{L}/\text{kPa}) = 7.30814 – 2367.155/(111.016 + T/K); \text{ temp range 445–508 K} \] (Antoine eq.-VII, Stephenson & Malanowski 1987)

10854 (calculated-UNIFAC activity coeff., Banerjee et al. 1990)
20136* (24.96°C, Hg manometer, measured range 9.95–49.97°C, Gracia et al. 1992)
20180* (recommended, Ruzicka & Majer 1994)

\[ \ln [(P/\text{kPa})(P\text{L}/\text{kPa})] = [1 – (T/K)/(T/K)] \cdot \exp(2.79797 – 2.022083 \times 10^{-3} \cdot (T/K) + 2.287564 \times 10^{-6} \cdot (T/K)^2); \] reference state at \( P_o = 101.325 \text{ kPa}, T_o = 341.863 \text{ K} \) (Cox equation, Ruzicka & Majer 1994)

\[ \log (P/\text{mmHg}) = 69.7378 – 3.6278 \times 10^{-1}/(T/K) – 23.927 \log (T/K) + 1.281 \times 10^{-2} \cdot (T/K) – 1.6844 \times 10^{-13} \cdot (T/K)^2; \] temp range 178–507 K (vapor pressure eq., Yaws 1994)

24938, 53982 (30, 50°C, VLE equilibrium data, Carmona et al. 2000)

Henry’s Law Constant (Pa m/mol at 25°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\text{AW}, C\text{AW}/C\text{A}, reported as exptl., Hine & Mookerjee 1975)
160000, 50590 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
190000 (calculated-P/C, Mackay & Shiu 1975, 1981; Bobra et al. 1979)
177060 (equilibrium cell-concen ratio-GC, Vejrosta et al. 1982)
173340* (equilibrium cell-concentration ratio-GC, measured range 14.52–34.9°C Jönsson et al. 1982)
103262, 135400, 172140, 215420, 261420 (15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
\[ \ln \left( 1/K_{AW} \right) = 21493.1/(T/K) + 59.299 \cdot \ln (T/K) – 414.193; \text{ temp range 15–35°C (least-square regression of equilibrium cell-concen ratio-GC measurements, Jönsson et al. 1982)} \]
77820* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
\[ \ln \left[ H/(atm_m^3/mol) \right] = 25.25 – 7530/(T/K); \text{ temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)} \]
130790 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
18600* (40°C, equilibrium headspace-GC, measured range 40–70°C, Kolb et al. 1992)
\[ \ln \left( 1/K_{AW} \right) = –28.60 + 8375/(T/K); \text{ temp range 40–70°C (equilibrium headspace-GC measurements, Kolb et al. 1992)} \]
163812 (EPICS-GC, Ryu & Park 1999)
65318 (20°C, selected from reported experimental values, Staudinger & Roberts 1996, 2001)
\[ \log K_{AW} = 12.150 – 3143/(T/K); \text{ (summary of literature data, Staudinger & Roberts 2001)} \]

Octanol/Water Partition Coefficient, log \( K_{OW} \):
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)
4.25 (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 \( K_{OA} \) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.55* (20.29°C, from GC-determined \( \gamma^\infty \) in octanol, measured range 20.29–50.28°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 BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO\(_3\) radical and \( k_{OOH} \) with O\(_3\) or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

\( k_{OO3P} = 9.30 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for reaction with O(3P) atoms (Herron & Huie 1973)
\( k_{OH} = (3.8 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \) at 305 K (relative rate method, Llyod et al. 1976)
\( k_{OH} = 5.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (Atkinson et al. 1979)
\( k_{OH} = (6.1 – 6.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 292–303 K, \( k_{OH} \) (calc) = 6.96 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 300 K (Darnall et al. 1978)
\( k_{OH} = 5.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \); \( k_{OO3P} = 9.3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for reaction with O(3P) atoms, at room temp. (abstraction mechanism, Gaffney & Levine 1979)
\( k_{OH} = (5.71 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 299 ± 2 K (relative rate method, Atkinson et al. 1982a)
\( k_{NO3} = (1.05 \pm 0.2) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 K (Atkinson et al. 1984a, Atkinson 1991)
\( k_{OH} = (5.70 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (relative rate, Atkinson et al. 1984c)
Aliphatic and Cyclic Hydrocarbons

- $k_{\text{OH}} = 5.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (relative rate, Atkinson & Aschmann 1984)
- $k_{\text{OH}} = 6.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 312 K in smog chamber (Nolting et al. 1988)
- $k_{\text{OH}}^* = 5.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1991, Altshuller 1991)
- $k_{\text{OH}} = 5.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 1.05 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljic & Güsten 1990)
- $k_{\text{OH}} = 5.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 10.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)
- $k_{\text{NO}_3} = 1.05 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 \pm 2 K (Atkinson 1991)
- $k_{\text{NO}_3}^{\text{exptl}} = 1.06 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3}^{\text{calc}} = 1.11 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 \pm 2 K (relative rate method, Aschmann & Atkinson 1995)
- $k_{\text{OH}}^* = 5.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 11 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)
- $k_{\text{OH}}^* = 5.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
- Air: photooxidation reaction $t_{\frac{1}{2}} = 2.4–24$ h in air, based on reaction rate constant of $3.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical (Darnall et al. 1976);
- atmospheric lifetime $\sim 25$ h, based on a rate constant of $5.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radicals in summer daylight (Altshuller 1991).

### TABLE 2.1.1.16.1
Reported aqueous solubilities of $n$-hexane at various temperatures

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<tr>
<th>Method</th>
<th>Temperature/°C</th>
<th>Solubility S/g·m⁻³</th>
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</thead>
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<tr>
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</tr>
<tr>
<td>14.0</td>
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<td>18.3</td>
<td>12.4</td>
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<td>69.7</td>
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<td>99.1</td>
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</table>

<table>
<thead>
<tr>
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<th>S/g·m⁻³</th>
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<th>S/g·m⁻³</th>
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(Continued)
TABLE 2.1.1.1.16.1 (Continued)

2.

<table>
<thead>
<tr>
<th>Tsonopoulos &amp; Wilson 1983</th>
<th>Shaw 1989a</th>
<th>IUPAC recommended</th>
<th>Mańczyński et al. 2004</th>
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FIGURE 2.1.1.1.16.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for n-hexane.
### TABLE 2.1.1.16.2
Reported vapor pressures of *n*-hexane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T(K)} \quad (1) \\
\log P = A - \frac{B}{C + t(°C)} \quad (2) \\
\log P = A - \frac{B}{C + T(K)} \quad (3) \\
\log P = A - \frac{B}{T(K)} - C \log (T/K) \quad (4) \\
\ln \left[ \frac{P(kPa)}{P_0(kPa)} \right] = [1 - \frac{T_o(K)}{T(K)}]\exp\{A_0 - A_1(T/K) + A_2(T/K)^2\} \quad (5) - Cox eq.
\]

1. Smyth & Engel 1929
   - **static-manometer**

<table>
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<td>24811</td>
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<tr>
<td>40</td>
<td>36757</td>
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<tr>
<td>50</td>
<td>53409</td>
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   bp/°C: 68.8

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   eq. 2 \( P/mmHg \)  
   \[
   A = 6.87776 \\
   B = 1171.530 \\
   C = 224.366 \\
   \text{temp range: 13–69.5°C} \\
   \]

2. Willingham et al. 1945
   - **ebulliometry**

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   bp/°C: 38.311

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3. Stull 1947
   - **summary of literature data**

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<tr>
<td>67.030</td>
<td>95992</td>
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   eq. 2 \( P/mmHg \)
   \[
   A = 6.87024 \\
   B = 118.72 \\
   C = 224.210 \\
   \text{bp/°C: 68.744} \\
   \]

4. Zwolinski & Wilhoit 1971
   - **selected values**

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   \( \Delta H_v/(kJ mol^{-1}) = \)
   at 25°C 31.55
   at bp 28.85

(Continued)
TABLE 2.1.1.1.16.2 (Continued)

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<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<th>P/Pa</th>
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<td>40996</td>
<td>34.95</td>
<td>30577</td>
<td>282.95</td>
<td>10000</td>
</tr>
<tr>
<td>-61.25</td>
<td>64.13</td>
<td>45.15</td>
<td>45289</td>
<td>39.93</td>
<td>37185</td>
<td>341.863</td>
<td>101325</td>
</tr>
<tr>
<td>-53.29</td>
<td>128</td>
<td>48.11</td>
<td>50476</td>
<td>44.96</td>
<td>45000</td>
<td>298.15</td>
<td>20180</td>
</tr>
<tr>
<td>-34.84</td>
<td>656</td>
<td>49.97</td>
<td>54028</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

-24.91 | 1264 | Antoine eq. |  |
-14.39 | 2560 | eq. 3 | P/mmHg |  |
-0.51 | 3120 | A | 6.6298 | Antoine eq. |  |
B | 1050.38 | eq. 3a | P/kPa |  |
mp/°C | -95.36 | C | 210.477 |  |
| | A | 13.74029 |  |
B | 2654.670 |  |

eq. 1a P/mmHg \( \Delta H_v/(kJ \cdot mol^{-1}) = 30.84 \)

A | 19.5553 |
B | 4292.8 |

FIGURE 2.1.1.1.16.2 Logarithm of vapor pressure versus reciprocal temperature for \( n \)-hexane.
### TABLE 2.1.1.16.3
Reported Henry’s law constants and octanol-air partition coefficients of *n*-hexane at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.52</td>
<td>103536</td>
<td>10</td>
<td>24115</td>
<td>40</td>
<td>18600</td>
<td>20.29</td>
</tr>
<tr>
<td>14.52</td>
<td>103090</td>
<td>15</td>
<td>41847</td>
<td>60</td>
<td>64410</td>
<td>20.29</td>
</tr>
<tr>
<td>15.0</td>
<td>103262</td>
<td>20</td>
<td>89470</td>
<td>70</td>
<td>237750</td>
<td>20.29</td>
</tr>
<tr>
<td>20.05</td>
<td>135426</td>
<td>25</td>
<td>77818</td>
<td>eq. 2</td>
<td>1/K_{AW}</td>
<td>20.29</td>
</tr>
<tr>
<td>20.05</td>
<td>136182</td>
<td>30</td>
<td>158067</td>
<td>eq. 2</td>
<td>1/K_{AW}</td>
<td>20.29</td>
</tr>
<tr>
<td>20.0</td>
<td>135403</td>
<td></td>
<td></td>
<td>eq. 2</td>
<td>1/K_{AW}</td>
<td>20.29</td>
</tr>
<tr>
<td>25</td>
<td>174565</td>
<td></td>
<td></td>
<td>eq. 4</td>
<td>H/(atm m³/mol)</td>
<td>7530</td>
</tr>
<tr>
<td>25</td>
<td>172140</td>
<td>A</td>
<td>25.25</td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>25</td>
<td>172140</td>
<td>B</td>
<td>7530</td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>30.2</td>
<td>215560</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>30.2</td>
<td>211937</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>30.0</td>
<td>215418</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>34.9</td>
<td>264034</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>34.9</td>
<td>256113</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7530</td>
</tr>
<tr>
<td>35.0</td>
<td>261424</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7530</td>
</tr>
</tbody>
</table>

*Henry's law constant*  

\[
\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a) \\
\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a) \\
\ln \left[ \frac{H}{(atm \cdot m^3/mol)} \right] = A - B/(T/K) \quad (3) \quad \log \left[ \frac{H}{(atm \cdot m^3/mol)} \right] = A - B/(T/K) \quad (4) \\
K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2 \quad (5) \\
\]

*FIGURE 2.1.1.16.3* Logarithm of Henry’s law constant versus reciprocal temperature for *n*-hexane.

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FIGURE 2.1.1.16.4 Logarithm of $K_{OA}$ versus reciprocal temperature for $n$-hexane.
Common Name: 2-Methylhexane
Synonym: isoheptane, ethylisobutylmethane
Chemical Name: 2-methylhexane
CAS Registry No: 591-76-4
Molecular Formula: C\textsubscript{7}H\textsubscript{16}; CH\textsubscript{3}CH(CH\textsubscript{3})CH\textsubscript{2}(CH\textsubscript{2})\textsubscript{2}CH\textsubscript{3}
Molecular Weight: 100.202

Melting Point (°C):
-118.2 (Lide 2003)

Boiling Point (°C):
90.04 (Lide 2003)

Density (g/cm\textsuperscript{3} at 20°C):
0.6786, 0.6744 (20°C, 25°C, Dreisbach 1959)
0.6786, 0.6548 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm\textsuperscript{3}/mol):
147.66, 148.58 (20°C, 25°C, calculated-density)
162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, $\Delta H_{\text{v}}$ (kJ/mol):
34.807, 30.669 (25°C, bp, Riddick et al. 1986)

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

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

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
2.54 (shake flask-GC, Price 1976)
3.51 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
8380 (calculated-Antoine eq. regression, temp range –40.4 to 90°C, Stull 1947)
9000 (25.518°C, ebulliometry, measured range 18.5–90.9°C, Forziati et al. 1949)

$\log (P/\text{mmHg}) = 6.87319 – 1236.026/(219.545 + t/°C)$; temp range (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)

8780 (calculated from determined data, Dreisbach 1959)

$\log (P/\text{mmHg}) = 6.87318 – 1236.026/(219.545 + t/°C)$; temp range 10–110°C (Antoine eq. for liquid state, Dreisbach 1959)

8780 (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

$\log (P/\text{mmHg}) = 5.87318 – 1236.026/(219.545 + t/°C)$; temp range –9.10 to 114.78°C (Antoine eq., Zwolinski & Wilhoit 1971)

8370 (interpolated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [–0.2185 \times 8538.7/(T/K)] + 8.055523$; temp range –40.4 to 90°C (Antoine eq., Weast 1972–73)
87778, 8785 (interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{Pa}) = -0.0031 – 1238.614/(219.867 + t/°C)$; temp range 18.5–90.9°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

$\log (P/\text{Pa}) = 6.06712 – 1270.535/(222.971 + t/°C)$; temp range 0–45°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

8790 (interpolated-Antoine eq., temp range –9 to 115°C, Dean 1985, 1992)

$\log (P/\text{mmHg}) = 6.87318 – 1236.026/(219.55 + t/°C)$; temp range –9 to 115°C (Antoine eq., Dean 1985, 1992)
8800 (lit. average, Riddick et al. 1986)

\[
\log (P/kPa) = 5.99612 - 1235.10/(219.469 + t/°C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

8790 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/kPa) = 6.00513 - 1240.11/(-53.123 + T/K); \text{ temp range 296–365 K (Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log (P/mmHg) = 54.1075 - 3.785 \times 10^3/(T/K) - 17.547 \log (T/K) + 8.2594 \times 10^{-3}(T/K) - 3.4967 \times 10^{-14}(T/K)^2; \text{ temp range 155–530 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m³/mol at 25°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)


\[
\ln [H/(kPa·m³/mol)] = 3608/(T/K) - 8.0; \text{ temp range 26.9–45°C (EPICS-GC, Hansen et al. 1993)}
\]

63856 (20°C, selected from reported experimental determined values, Staudinger & Roberts 2001)

\[
\log K_{AW} = -4.274 + 1669/(T/K) \text{ (summary of literature data, Staudinger & Roberts 2001)}
\]

Octanol/Water Partition Coefficient, log K_{OW}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}

with NO_{3} radical and k_{O3} with O_{3} or as indicated, *data at other temperatures see reference:

\[
k_{OH} = 6.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Atkinson 1990, 1991)}
\]

\[
k_{OH} = 6.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with atmospheric lifetime of 25 h in summer daylight (Altshuller 1990)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of 6.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} with hydroxyl radicals and an estimated lifetime of 25 h in summer daylight (Altshuller 1990).

**TABLE 2.1.1.17.1**

Reported Henry’s law constants of 2-methylhexane at various temperatures

<table>
<thead>
<tr>
<th>Hansen et al. 1993</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>EPICS-GC</strong></td>
</tr>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>26.9</td>
</tr>
<tr>
<td>35.0</td>
</tr>
<tr>
<td>45.0</td>
</tr>
</tbody>
</table>

\[
\ln [H/(Pa·m³/mol)] = A - B/(T/K) \text{  eq. 4 H/(kPa m³/mol)}
\]

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>−8  ± 3.53</td>
<td>−3608 ± 1088</td>
</tr>
</tbody>
</table>
2.1.1.1.18 3-Methylhexane

Common Name: 3-Methylhexane
Synonym: ethylmethylpropylmethane
Chemical Name: 3-methylhexane
CAS Registry No: 589-34-4
Molecular Formula: C_{7}H_{16}; CH_{3}CH_{2}CH(CH_{3})(CH_{2})_{2}CH_{3}
Molecular Weight: 100.202
Melting Point (°C):
-119.4 (Riddick et al. 1986; Lide 2003)
Boiling Point (°C):
92 (Lide 2003)
Density (g/cm³ at 20°C):
0.6860 (Weast 1984)
0.6871, 0.6830 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
145.83, 146.71 (calculated-density)
162.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, Δ_H^v (kJ/mol):
35.087, 30.79 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, Δ_H^fus (kJ/mol):
Entropy of Fusion, Δ_S^fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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 (0.25°C, calculated-recommended liquid-liquid equilibrium LLE data, Mańczyński et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
7782 (Antoine eq. regression, temp range –39 to 91.9°C Stull 1947)
7702 (23.662°C, ebulliometry, measured range 19.915–92.737°C, Forziati et al. 1949)
log (P/mmHg) = 6.86754 – 1240.196/(219.223 + t°C); temp range 19.9–92.7°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
8210 (calculated from determined data, Dreisbach 1959)
log (P/mmHg) = 6.86764 – 1240.196/(219.223 + t°C); temp range 10–130°C (Antoine eq. for liquid state, Dreisbach 1959)
8213 (interpolated-Antoine eq., temp range –7.90 to 116.73°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.86764 – 1240.196/(219.223 + t°C); temp range –7.90 to 116.73°C (Antoine eq., Zwolinski & Wilhoit 1971)
7772 (interpolated-Antoine eq., temp range –39.0 to 91.9°C, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 8596.3/(T/K)] + 8.065472; temp range –39.0 to 91.9°C (Antoine eq., Weast 1972–73)
8212 (interpolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 5.99489 – 1241.528/(219.375 + t°C); temp range 20–92.74°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublík et al. 1984)
8210 (interpolated-Antoine eq., temp range –8 to 117°C Dean 1985, 1992)
log (P/mmHg) = 6.86764 – 1240.196/(219.223 + t°C); temp range –8 to 117°C (Antoine eq., Dean 1985, 1992)
8300 (lit. average, Riddick et al. 1986)
log (P/kPa) = 5.98993 – 1238.88/(219.10 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
8215 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log \left( \frac{P}{kPa} \right) = 5.9926 - \frac{1239.57}{-53.979 + T/K}; \text{ temp range } 289-366 \text{ K (Antoine eq., Stephenson & Malanowski 1987)}
\]
\[
\log \left( \frac{P}{\text{mmHg}} \right) = 35.2535 - 2.931 \times 10^3/(T/K) - 9.667 \log (T/K) - 5.2026 \times 10^{-11} \cdot (T/K)^2; \text{ temp range } 154-535 \text{ K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C):

172000 \quad \text{(recommended, Mackay & Shiu 1981)}
312170 \quad \text{(calculated-P/C, Eastcott et al. 1988)}
311620 \quad \text{(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)}

Octanol/Water Partition Coefficient, \( \log K_{ow} \):

Octanol/Air Partition Coefficient, \( \log K_{oa} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\text{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO3 radical and \( k_{O3} \) with O3 or as indicated, \*data at other temperatures see reference:

\( k_{OH} = 7.20 \times 10^{-12} \) cm^3 molecule^-1 s^-1 at 298 K (Atkinson 1990, 1991)

\( k_{OH} = 7.20 \times 10^{-12} \) cm^3 molecule^-1 s^-1 with a calculated atmospheric lifetime of 20 h during summer daylight (Altschuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric \( t_\text{1/2} \) ~ 2.4–24 h for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant of \( 7.20 \times 10^{-12} \) cm^3 molecule^-1 s^-1 with hydroxyl radical and an estimated lifetime of 20 h during summer daylight (Altschuller 1991).
2.1.1.1.19  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: C\(_9\)H\(_{20}\), (CH\(_3\))\(_3\)CCH\(_2\)CH\(_2\)CH(CH\(_3\))\(_2\)

Molecular Weight: 128.255

Melting Point (°C):

-105.7 (Lide 2003)

Boiling Point (°C):

124.09 (Lide 2003)

Density (g/cm\(^3\) at 25°C):

- 0.7072 (Weast 1984)
- 0.7072, 0.7032 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)

Molar Volume (cm\(^3\)/mol):

- 181.3, 182.4 (20°C, 25°C, calculated-density)
- 207.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):

- 40.175, 33.76 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):

- 6.192 (Riddick et al. 1986)

Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):

- Calculated-recommended liquid-liquid equilibrium LLE data, Mańczyński et al. 2004

Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):

- 1.15 (shake flask-GC, McAuliffe 1966)
- 0.79; 0.54, 0.54 (0; 25°C, shake flask-GC, calculated-group contribution, Polak & Lu 1973)
- 0.80, 0.80 (0, 25°C, IUPAC recommended best value, Shaw 1989b)
- 0.613 (calculated-recommended liquid-liquid equilibrium LLE data, Mańczyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

- \(\log (P/mmHg) = 6.83532 - 1324.049/(210.737 + t/°C)\); temp range 46.1–125.0°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
- 2212 (extrapolated-Antoine eq., Dreisbach 1959)
- \(\log (P/mmHg) = 6.83531 - 1324.059/(210.737 + t/°C)\); temp range 35–145°C (Antoine eq. for liquid state, Dreisbach 1959)
- 2210 (interpolated-Antoine eq., temp range 16.17–151.1°C, Zwolinski & Wilhoit 1971)
- \(\log (P/mmHg) = 6.83531 - 1324.049/(210.737+C + t/°C)\); temp range 16.17–151.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 2216 (static method-inclined piston manometer, measured range –35 to 30°C, Osborn & Douslin 1964)
- 2207 (extrapolated-Antoine eq., Boulik et al. 1984)
- \(\log (P/kPa) = 5.96385 - 1326.27/(212.991 + t/°C)\); temp range 46.14–126.05°C (Antoine eq. from reported expctl. data of Forziati et al. 1949, Boulik et al. 1984)
- 2207 (extrapolated-Antoine eq., temp range 46 to 125°C Dean 1985, 1992)
- \(\log (P/mmHg) = 6.83775 - 1325.54/(210.91 + t/°C)\); temp range 46–125°C (Antoine eq., Dean 1985, 1992)
- 2216 (lit. average, Riddick et al. 1986)
- \(\log (P/kPa) = 5.96021 - 1324.049/(210.737 + t/°C)\); temp range not specified (Antoine eq., Riddick et al. 1986)
- 2218 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
- \(\log (P_{L}/kPa) = 6.99253 - 1243.85/(60.158 + T/K)\); temp range 288–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/L/kPa) = 6.25179 – 1471.621/(-48.901 + T/K); temp range 238–293 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.8816 – 2.6422 × 10^3/(T/K) + 23.902·log (T/K) – 1.5376 × 10^{-2}·(T/K) + 7.7931 × 10^{-6}·(T/K)^2;
temp range 167–568 K (vapor pressure eq., Yaws 1994)

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

Octanol/Water Partition Coefficient, log $K_{ow}$:
4.63 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
4.46 (calculated-molar volume $V_M$, Wang et al. 1992)

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants and Half-Lives:

Half-Lives in the Environment:
2.1.1.20  n-Heptane

Common Name: n-Heptane
Synonym: heptane
Chemical Name: n-heptane
CAS Registry No: 142-82-5
Molecular Formula: C₇H₁₆, CH₃(CH₂)₅CH₃
Molecular Weight: 100.202
Melting Point (°C): –90.55 (Lide 2003)
Boiling Point (°C): 98.4 (Dreisbach 1959; Weast 1972–73; Lide 2003)
Density (g/cm³ at 20°C):
- 0.6837 (Weast 1972–73)
- 0.6837, 0.6795 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
- 146.6, 147.5 (20°C, 25°C, calculated-density)
- 162.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
- 36.55, 31.7 (25°C, bp, Riddick et al. 1986)
- 36.57 (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
- 14.037 (Riddick et al. 1986)
- 14.04 (Chickos et al. 1999)
Entropy of Fusion, ΔSₘₙ (J/mol K):
- 76.9, 81.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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 (15.5°C, shake flask-cloud point, Fühner 1924)
- 150 (radiotracer method, Black et al. 1948)
- 15.0 (16°C, shake flask-cloud point, Durand 1948)
- 2.93 (shake flask-GC, McAuliffe 1963, 1966)
- 11.0* (22°C, cloud point, measured range 295–355 K at 17–55 MPa, Connolly 1966)
- 2.66* (shake flask-GC, measured range 4.3–45°C, Nelson & De Ligny 1968)
- 4.39; 3.37* (0, 25°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°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. γ and KOW, Tewari et al. 1982b)
- 2.51* (vapor saturation-GC, measured range 15–40°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°C, Shaw 1989)

ln x = –396.93979 + 17232.298/(T/K) + 56.95927·ln (T/K), temp range 290–400 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, Mączyński et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

5520*  
(22.7°C, static-manometer, measured range 22.7–98.4°C, Smyth & Engel 1929)

6370*  
(25.9°C, ebulliometry, measured range 25.9–99.3°C, Willingham et al. 1945)

log (P/mmHg) = 6.90342 – 1268.636/(216.951 + t/°C); temp range 25.9–99.3°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)

5795*  
(calculated-Antoine eq. regression, temp range –34 to 98.4°C Stull 1947)

6110  
(calculated from determined data, Dreisbach 1959)

5080*  
(22.46°C, gas saturation, measured range –87.85 to 22.46°C, Carruth & Kobayashi 1973)

6037, 6057  
(static method-differential pressure gauge, Bissell & Williamson 1975)

5826, 5958, 6090  
(interpolated-Antoine eq., temp range 15–155°C (Antoine eq. for liquid state, Dreisbach 1959)

6090  
(interpolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.02701 – 1167.592/(216.796 + t/°C); temp range 25.92–99.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 4.38001 – 668.768/(159.522 + t/°C); temp range –87.85 to 22.4°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°C Dean 1985, 1992)

log (P/mmHg) = 6.98677 – 1264.90/(216.54 + t/°C); temp range –2 to 124°C (Antoine eq., Dean 1985, 1992)

6090  
(literature average, Riddick et al. 1986)

log (P/kPa) = 6.02167 – 1264.90/(216.44 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

6110  
(interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 6.02633 – 1265.83/(–56.054 + T/K); temp range 297–375 K (Antoine eq., Stephenson & Malanowski 1987)

6102*  
(recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_o/kPa)] = [1 – (T/K)/(T_o/K)]·exp{2.86470 – 2.113204 × 10–3·(T/K) + 2.250991 × 10–6·(T/K)2}; reference state at P_o = 101.325 kPa, T_o = 371.552 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 65.0257 – 3.8188 × 10³/(T/K) –21.684·log (T/K) + 1.0387 × 10–2·(T/K) + 1.0206 × 10–14·(T/K)²; temp range 183–540 K (vapor pressure eq., Yaws 1994)

12309  
(40°C, average value, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)

7811, 18869  
(30, 50°C, VLE equilibrium data, Carmona et al. 2000)

62503*  

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

206200  
(calculated-1/KAW, CW/CA, 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(15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl data, Jönsson et al. 1982)
\[ \ln \left( \frac{1}{K_{AW}} \right) = \frac{23748.4}{(T/K)} + 64.927 \ln \left( \frac{T}{K} \right) - 454.172; \text{temp range 15–35°C (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)} \]

\[ 273400 \text{ (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)} \]

\[ 91294^* \text{ (26°C, EPICS-GC, measured range 26–45°C, Hansen et al. 1993)} \]

\[ \ln \left( \frac{H}{(kPa \cdot m^3/mol)} \right) = -3730/(T/K) + 17.0; \text{temp range 26–45°C (EPICS-GC, Hansen et al. 1993)} \]

\[ 220825 \text{ (EPICS-GC, Ryu & Park 1999)} \]

\[ 68000 \text{ (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)} \]

\[ \log K_{AW} = 6.532 - 1491/(T/K); \text{(summary of literature data, Staudinger & Roberts 2001)} \]

### Octanol/Water Partition Coefficient, \( K_{OW} \):

- 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 ± 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, \( K_{OA} \) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.:

- 3.05* (20.29°C, from GC-determined \( \gamma^\infty \) in octanol, measured range 20.29–50.28°C Gruber et al. 1997)
- 2.95 (calculated-measured \( \gamma^\infty \) in pure octanol and vapor pressure P, Abraham et al. 2001)

### Bioconcentration Factor, \( BCF \):

### Sorption Partition Coefficient, \( K_{OC} \):

### Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

#### Volatilization:

#### Photolysis:

#### Oxidation: rate constant \( k \), for reaction with \( OH \) radical, \( k_{OH} \) with \( NO_3 \) radical and \( k_{\text{O}_3} \) with \( O_3 \) or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[ k_{OH} = (7.30 \pm 0.17) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \pm 2 \text{ K (relative rate method, Atkinson et al. 1982a, 1984c)} \]

\[ k_{NO_3} = 1.36 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1988,1990)} \]

\[ k_{OH} = 7.52 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 312 \text{ K in smog chamber (Nolting et al. 1988)} \]

\[ k_{OH} = 7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989, 1991)} \]

\[ k_{OH} = 7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, } k_{NO_3} = 1.36 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (Atkinson 1990)} \]

\[ k_{OH} = 7.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{KNO_3} = 1.36 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Sabljic & Güsten 1990)} \]

\[ k_{OH} = 7.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K, with a calculated atmospheric lifetime of 19 h during summer daylight hours (Altschuller 1991)} \]

\[ k_{NO_3} = (1.34 - 1.37) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (Atkinson 1991)} \]

\[ k_{NO_3}(\text{exptl}) = (1.36, 1.38) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3}(\text{recommended}) = 1.37 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]

\[ k_{NO_3}(\text{calc}) = 1.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (relative rate method, Aschmann & Atkinson 1995)} \]

\[ k_{OH} = 7.02 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 15 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)} \]

### Hydrolysis:

### Biodegradation:
### TABLE 2.1.1.20.1
Reported aqueous solubilities of *n*-heptane at various temperatures

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<td>t/°C</td>
<td>S/g·m⁻³</td>
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\[ \Delta H_{\text{sol}}/(kJ \text{ mol}^{-1}) = -2.43 \]
![Figure 2.1.1.1.20.1](image)

**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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\ln \left[ \frac{(P/kPa)/(P_0/kPa)}{1 - (T_0/K)/(T/K)} \right] &= \left[ A_0 - A_1(T/K) + \frac{A_2}{(T/K)^2} \right] \quad (5) - \text{Cox eq.} 
\end{align*}
\]

1. Smyth & Engel 1929
   - static method-manometer

   \[
   \begin{array}{ccc}
   t/°C & P/Pa & t/°C & P/Pa \\
   22.7 & 5520 & 25.925 & 6370 \\
   30.0 & 7759 & 29.699 & 7665 \\
   30.3 & 7839 & 33.024 & 8977 \\
   38.4 & 11466 & 36.017 & 10311 \\
   50.0 & 18812 & 38.822 & 11700 \\
   51.2 & 19998 & 42.599 & 13821 \\
   61.2 & 29331 & 46.929 & 16604 \\
   69.5 & 40183 & 51.320 & 19920 \\
   79.5 & 55955 & 55.394 & 23443 \\
   98.4 & 101325 & 60.862 & 28950 \\
   \text{mp/°C} & -90.5 & 78.160 & 53647 \\
   \text{bp/°C} & 98.4 & 84.823 & 66749 \\
   \end{array}
   \]

2. Willingham et al. 1945
   - ebulliometry

   \[
   \begin{array}{ccc}
   t/°C & P/Pa & t/°C & P/Pa \\
   25.925 & 6370 & -34.0 & 133.3 \\
   29.699 & 7665 & -12.7 & 666.6 \\
   33.024 & 8977 & -2.1 & 1333 \\
   36.017 & 10311 & 9.5 & 2666 \\
   38.822 & 11700 & 22.3 & 5333 \\
   42.599 & 13821 & 30.6 & 7999 \\
   46.929 & 16604 & 41.8 & 13332 \\
   51.320 & 19920 & 58.7 & 26664 \\
   55.394 & 23443 & 78.0 & 53329 \\
   60.862 & 28950 & 98.4 & 101325 \\
   78.160 & 53647 & 71.930 & 43326 & \text{mp/°C} -90.6 \\
   84.823 & 66749 & 84.823 & 53647 \\
   92.053 & 83706 & 98.4 & 100689 \\
   97.154 & 97590 & 97.154 & 97590 \\
   97.702 & 99186 & 97.702 & 99186 \\
   98.207 & 100689 & 98.207 & 100689 \\
   \end{array}
   \]

3. Stull 1947
   - summary of literature data

   \[
   \begin{array}{ccc}
   t/°C & P/Pa & t/°C & P/Pa \\
   -34.0 & 133.3 & -2.1 & 1333 \\
   -12.7 & 666.6 & 9.5 & 2666 \\
   -2.1 & 1333 & 22.3 & 5333 \\
   -12.7 & 666.6 & 30.6 & 7999 \\
   -2.1 & 1333 & 41.8 & 13332 \\
   -12.7 & 666.6 & 58.7 & 26664 \\
   -2.1 & 1333 & 78.0 & 53329 \\
   -12.7 & 666.6 & 98.4 & 101325 \\
   -2.1 & 1333 & 71.930 & 43326 & \text{mp/°C} -90.6 \\
   -12.7 & 666.6 & 88.4 & 53329 \\
   -2.1 & 1333 & 97.154 & 97590 \\
   -12.7 & 666.6 & 97.702 & 99186 \\
   -2.1 & 1333 & 98.207 & 100689 \\
   -12.7 & 666.6 & 98.207 & 100689 \\
   \end{array}
   \]

4. Forziati et al. 1949
   - ebulliometry

   \[
   \begin{array}{ccc}
   t/°C & P/Pa & t/°C & P/Pa \\
   26.030 & 6425 & 29.813 & 7717 \\
   33.108 & 9013 & 36.105 & 10352 \\
   38.901 & 11740 & 42.680 & 13866 \\
   46.987 & 16659 & 51.373 & 19966 \\
   55.442 & 23499 & 60.902 & 29003 \\
   65.916 & 34948 & 71.966 & 43386 \\
   78.202 & 53270 & 84.856 & 66815 \\
   92.678 & 83769 & 97.180 & 97663 \\
   97.728 & 99257 & 97.728 & 99257 \\
   98.237 & 100758 & 98.237 & 100758 \\
   \end{array}
   \]

(Continued)
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2. Zwolinski & Wilhoit 1971

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<td>6.89385</td>
<td>eq. 5</td>
<td>P/kPa</td>
</tr>
<tr>
<td>B</td>
<td>1264.37</td>
<td>A</td>
<td>2.86470</td>
</tr>
<tr>
<td>C</td>
<td>216.636</td>
<td>eq. 3</td>
<td>P/kPa</td>
</tr>
<tr>
<td>bp/°C</td>
<td>98.429</td>
<td>A</td>
<td>2.113204 × 10⁻³</td>
</tr>
<tr>
<td>∆H/(/kJ mol⁻¹) =</td>
<td>with reference state at</td>
<td>2.250991 × 10⁻⁶</td>
<td>386.826</td>
</tr>
<tr>
<td>at 25°C</td>
<td>36.55</td>
<td>P/kPa</td>
<td>293.069</td>
</tr>
<tr>
<td>at bp</td>
<td>31.70</td>
<td>101.325</td>
<td>383.069</td>
</tr>
</tbody>
</table>

see ref. for complete set of data
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

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \quad (1) \\
\log K_{AW} &= A - B/(T/K) \quad (1a) \\
\ln (1/K_{AW}) &= A - B/(T/K) \quad (2) \\
\log (1/K_{AW}) &= A - B/(T/K) \quad (2a) \\
\ln (k_H/atm) &= A - B/(T/K) \quad (3) \\
\ln [H/(Pa m^3/mol)] &= A - B/(T/K) \quad (4) \\
\ln [H/(atm·m^3/mol)] &= A - B/(T/K) \quad (4a) \\
K_{AW} &= A - B·(T/K) + C·(T/K)^2 \quad (5)
\end{align*}
\]

Henry’s law constant

<table>
<thead>
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<th></th>
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<tr>
<td>equilibrium cell-GC</td>
<td>EPICS-GC</td>
<td>GC det’d activity coefficient</td>
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<tr>
<td>( t/°C )</td>
<td>( H/(Pa m^3/mol) )</td>
<td>( t/°C )</td>
</tr>
<tr>
<td>15.0</td>
<td>136118*</td>
<td>26.0</td>
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<tr>
<td>15.3</td>
<td>140244</td>
<td>35.8</td>
</tr>
<tr>
<td>15.3</td>
<td>136260</td>
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<td>20.0</td>
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<td>20.05</td>
<td>190443</td>
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<td>35.05</td>
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<td>34.83</td>
</tr>
</tbody>
</table>

* interpolated data

Figure 2.1.1.20.2 Logarithm of vapor pressure versus reciprocal temperature for n-heptane.
FIGURE 2.1.1.20.3 Logarithm of Henry's law constant versus reciprocal temperature for $n$-heptane.

FIGURE 2.1.1.20.4 Logarithm of $K_{OA}$ versus reciprocal temperature for $n$-heptane.
2.1.1.1.21 2-Methylheptane

Common Name: 2-Methylheptane
Synonym:
Chemical Name: 2-methylheptane
CAS Registry No: 592-27-8
Molecular Formula: C₈H₁₈; CH₃CH(CH₃)(CH₂)₄CH₃
Molecular Weight: 114.229
Melting Point (°C):
-109.02 (Lide 2003)
Boiling Point (°C):
117.66 (Lide 2003)
Density (g/cm³ at 20°C):
0.698 (Lide 2003)
Molar Volume (cm³/mol):
163.7 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
185.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
39.68, 33.60 (25°C, normal bp, Dreisbach 1959)
Enthalpy of Fusion, ΔHfus (kJ/mol):
11.92 (Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
72.62, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.95, 4.55 (quoted, calculated-molar volume VM, 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°C and reported temperature dependence equations):
log (P/mmHg) = 6.91737 – 1337.468/(213.693 + t°C); temp range 41.7–118.5°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
2620 (calculated-Antoine eq. regression, temp range –21 to 117.6°C Stull 1947)
6386 (23.4°C, Nicolini & Laffitte 1949)
2748 (extrapolated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.91735 – 1337.468/(213.693 + t°C); temp range 35–150°C (Antoine eq. for liquid state, Dreisbach 1959)
2748 (interpolated-Antoine eq., temp range 12.3–143.8°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.91735 – 1337.468/(213.693 + t°C); temp range 12.3–143.8°C (Antoine eq., Zwolinski & Wilhoit 1971)
2620 (interpolated-Antoine eq., temp range –21–117.6°C, Weast 1972–73)
log (P/mmHg) = [–0.2185 × 9362.0/(T/K)] + 8.154424; temp range –21–117.6°C (Antoine eq., Weast 1972–73)
2732, 6850 (calculated-Antoine eq., Boublik et al. 1973, 1984)
log (P/mmHg) = 6.88814 – 1319.539/(211.625 + t°C); temp range 41–118.5°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1973)
log (P/mmHg) = 6.85999 – 1313.125/(230.02 + t°C); temp range 23.4–75°C (Antoine eq. from reported exptl. data of Nicolini & Laffitte 1949, Boublik et al. 1973)
1161 (10°C, static method-inclined piston manometer, measured range –40 to 10°C, Osborn & Douslin 1974)
log \( \frac{P}{mmHg} = 6.91735 - \frac{1337.47}{213.69 + t/°C} \); temp range 42–119°C (Antoine eq., Dean 1985, 1992)

log \( \frac{P}{kPa} = 6.05858 - \frac{1346.996}{-30.648 + T/K} \); temp range 285–392 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log \( \frac{P}{kPa} = 6.81199 - \frac{1703.6}{-30.648 + T/K} \); temp range 233–286 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( \frac{P}{mmHg} = 37.693 - 3.2611 \times 10^{-3}/(T/K) - 10.391 \cdot \log (T/K) - 1.0524 \times 10^{-12} \cdot (T/K)^2 \); temp range 164–560 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

369,880 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

3.91 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

4.04 (calculated-V M, Wang et al. 1992)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

V olatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with \( NO_3 \) radical and \( k_{O3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference:

\( k_{OH}(calc) = 8.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) (SAR structure reactivity relationship, Atkinson 1987)

\( k_{OH} = 8.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with a calculated atmospheric lifetime \( \tau = 17 \text{ h} \) during summer daylight hours (Altshuller 1991).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of \( 8.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with hydroxyl radical and an estimated lifetime of 17 h during summer daylight (Altshuller 1991).
2.1.1.22 3-Methylheptane

Common Name: 3-Methylheptane
Synonym:
Chemical Name: 3-methylheptane
CAS Registry No: 589-81-1
Molecular Formula: C₈H₁₈; CH₃CH₂CH(CH₃)(CH₂)₃CH₃
Molecular Weight: 114.229
Melting Point (°C):
-120.48 (Lide 2003)
Boiling Point (°C):
118.9 (Lide 2003)
Density (g/cm³ at 20°C):
0.7075 (Weast 1984)
0.7058, 0.7018 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
161.4 (20°C, calculated-density, Stephenson & Malanowski 1987)
185.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
39.83, 34.08 (25°C, normal bp, Dreisbach 1959)
Enthalpy of Fusion, ∆H₅ₐ (kJ/mol):
11.38 (Dreisbach 1959)
11.7 (Chickos et al. 1999)
Entropy of Fusion, ∆S₅ₐ (J/mol K):
76.6, 64.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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, Mączyński et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
\[ \log (P/\text{mmHg}) = 6.89945 - 1313.530/(212.414 + t/°C); \text{ temp range 42.7–119.8°C} \text{ (Antoine eq. from exptl. data, ebulliometry, manometer, Willingham et al. 1945)} \]
2610 (calculated from determined data, Dreisbach 1959)
\[ \log (P/\text{mmHg}) = 6.89944 - 1313.530/(212.414 + t/°C); \text{ temp range 30–150°C} \text{ (Antoine eq. for liquid state, Dreisbach 1959)} \]
2600 (interpolated-Antoine eq., temp range 13.3–145.2°C, Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 6.89944 - 1313.530/(212.414 + t/°C); \text{ temp range 13.3–145.2°C} \text{ (Antoine eq., Zwolinski & Wilhoit 1971)} \]
2466 (interpolated-Antoine eq., temp range −19.8 to 118.9°C, Weast 1972–73)
\[ \log (P/\text{mmHg}) = [−0.2185 \times 9432.0/(t/K)] + 8.179407; \text{ temp range −19.8 to 118.9°C} \text{ (Antoine eq., Weast 1972–73)} \]
1486 (15°C, static method-inclined piston manometer, measured range −35 to 15°C, Osborn & Douslin 1974)
2600, 3232 (quoted, calculated-bp, Mackay et al. 1982)
2600 (extrapolated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{Pa}) = 6.01647 - 1326.329/(211.776 + t/°C); \text{ temp range 42.67–119.8°C} \text{ (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)} \]
2605 (extrapolated, Antoine eq., temp range 43–120°C Dean 1985, 1992)
\[ \log (P/\text{mmHg}) = 6.89944 - 1313.530/(212.414 + t/°C); \text{ temp range 43–120°C} \text{ (Antoine eq., Dean 1985, 1992)} \]
log \( P \) (kPa) = 6.02047 – 1329.42/(–60.945 + T/K); temp range 286–393 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log \( P \) (kPa) = 6.50909 – 1567.45/(–40.786 + T/K); temp range 238–286 K (Antoine eq.-II, Stephenson & Malanowski 1987)

\[
\log (P/\text{mmHg}) = 52.8828 – 3.6231 \times 10^3/(T/K) –16.804 \log (T/K) + 7.1828 \times 10^{-3} \cdot (T/K) + 7.4077 \times 10^{-14} \cdot (T/K)^2;
\]

temp range 153–564 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/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, \( \log K_{ow} \):

Octanol/Air Partition Coefficient, \( \log K_{oa} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_h \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO₃ radical and \( k_{O_3} \) with O₃ or as indicated, *data at other temperatures see reference:

\[
k_{OH}(\text{calc}) = 8.90 \times 10^{-12} \, \text{cm}^3 \text{molecule}^{-1} \, \text{s}^{-1} \text{ at room temp. (SAR, Atkinson 1987)}
\]

\[
k_{OH} = 8.90 \times 10^{-12} \, \text{cm}^3 \text{molecule}^{-1} \, \text{s}^{-1} \text{ with a calculated atmospheric lifetime } \tau = 16 \text{ h during summer daylight hours (Altshuller 1991)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant of \( 8.90 \times 10^{-12} \, \text{cm}^3 \text{molecule}^{-1} \, \text{s}^{-1} \) 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: C₈H₁₈; CH₃(CH₂)₆CH₃
Molecular Weight: 114.229
Melting Point (°C): 
   –56.82  (Lide 2003)
Boiling Point (°C): 
   125.67  (Lide 2003)
Density (g/cm³ at 20°C):
   0.7027, 0.6886  (20°C, 25°C, Riddick et al. 1986)
   0.70256  (20°C, digital precision densimeter, Dejoz et al. 1996)
Molar Volume (cm³/mol):
   162.6, 165.8 (20°C, 25°C, calculated-density)
   185.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
   41.49, 34.431  (25°C, bp, Riddick et al. 1986)
   41.56  (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
   20.74  (Dreisbach 1959; Riddick et al. 1986; Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
   95.86, 91.1  (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Nelson & De Ligny 1968)
0.700  (shake flask-GC, Krznoschhekova & Gubergrits 1973)
1.35; 0.85  (0, 25°C, shake flask-GC, Polak & Lu 1973)
0.431*  (shake flask-GC, measured range 25149.5°C, Price 1976)
0.615*  (vapor saturation-GC, measured range 15–35°C, Jönsson et al. 1982)
1.103  (generator column-GC, Tewari et al. 1982a; Wasik et al. 1982)
1.56  (calculated-activity coeff. and Kᵣₒₒ, 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*  (37.75°C, shake flask-GC, measured range 37.75–280°C, pressure range 0.0103–8.86 MPa, Heidmen et al. 1985)

ln x = –343.1497 + 13862.49/(T/K) + 49.24600·ln (T/K); temp range 37.75–280°C (shake flask-GC, Heidman et al. 1985)

0.884, 0.949  (20°C, shake flask-GC, Burris & MacIntyre 1986)
1.250  (shake flask-purge and trap-GC, Coutant & Keigley 1988)
0.71*  (recommended, temp range 0–100°C, IUPAC Solubility Data Series, Shaw 1989)

ln x = –415.7563 + 17975.386/(T/K) + 59.55451·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

0.774*  (29.9°C, shake flask-solid extraction-GC/FID, measured range 29.9–183°C, Marche et al. 2003)

ln x = –362.618 + 14904.474/(T/K) + 52.067·ln (T/K); temp range 29.9–183°C (shake flask-solid extraction-GC/FID measurements, Marche et al. 2003)
0.635* (calculated-liquid-liquid equilibrium LLE data, temp range 288.2–36.1 K, Mączyński et al. 2004)
0.807 (24.9°C, generator column-GC/FID, measured range 10–45°C, Sarraute et al. 2004)

Vapor Pressure (Pa at 25°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* (3.7°C, static-McLeod gauge, measured range –9.31 to 3.7°C, Linder 1931)
- 7670* (52.972°C, ebulliometry, measured range 52.972–126.570°C, Willingham et al. 1945)
- log (P/mmHg) = 6.92377 – 1355.126/(209.517 + t/°C); temp range 52.9–126.6°C (Antoine eq. from exp. data, ebulliometry-manometer, Willingham et al. 1945)
- 1777* (calculated-Antoine eq. regression, temp range –14 to 125.6°C, Stull 1947)
- 1870 (calculated from determined data, Dreisbach 1959)
- log (P/mmHg) = 6.92377 – 1355.126/(209.517 + t/°C); temp range 40–155°C (Antoine eq. for liquid state, Dreisbach 1959)
- 1885* (interpolated-Antoine eq., temp range 19.2–152.1°C, Zwolinski & Wilhoit 1971)
- log (P/mmHg) = 6.91868 – 1351.99/(209.15 + t/°C); temp range 19–152°C (Antoine eq., Dean 1985, 1992)
- log (P/kPa) = 6.04231 – 1351.491/(–64.014 + T/K); temp range 297–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P/kPa) = 6.16936 – 1440.32/(–52.894 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/kPa) = 7.66614 – 7.66614/(159.091 + T/K); temp range 506–569 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- 1825 (interpolated-Antoine eq., temp range 19.2–152°C, Dean 1985, 1992)
- log (P/kPa) = 6.04394 – 1351.938/(209.12 + t/°C); temp range 52.93–126.57°C (Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P/kPa) = 7.90115 – 2238.9/(–4.53 + T/K); temp range 216–278 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/kPa) = 6.16936 – 1440.32/(–52.894 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/kPa) = 6.23406 – 1492.068/(–45.851 + T/K); temp range 428–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 7.90115 – 2238.9/(–4.53 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 6.04394 – 1351.938/(209.12 + t/°C); temp range 52.93–126.57°C (Antoine eq.-I, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 7.90115 – 2238.9/(–4.53 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 6.16936 – 1440.32/(–52.894 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 6.23406 – 1492.068/(–45.851 + T/K); temp range 428–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 7.66614 – 7.66614/(159.091 + T/K); temp range 506–569 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 7.90115 – 2238.9/(–4.53 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 6.16936 – 1440.32/(–52.894 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 6.23406 – 1492.068/(–45.851 + T/K); temp range 428–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 7.66614 – 7.66614/(159.091 + T/K); temp range 506–569 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- log (P/L/kPa) = 7.90115 – 2238.9/(–4.53 + T/K); temp range 216–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°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 AW, CW/CA, reported as exp. 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* (25.1°C, equilibrium cell-concentration ratio-GC, measured range 14.8–34.92°C, Jönsson et al. 1982)
180130, 253880, 344280, 458250, 595800 (15, 20, 25, 30, 35°C, calculated-temp dependence eq. derived from exptl. data, Jönsson et al. 1982)
\[
\ln \left( \frac{1}{K_{AW}} \right) = \frac{26003.7}{(T/K)} + 70.571 \cdot \ln \left( \frac{T}{K} \right) - 494.151; \text{ temp range: } 15–35°C \text{ (least-square regression of equilibrium cell-concn ratio-GC measurements, Jönsson et al. 1982)}
\]
324200 (calculated-P/C, Lyman et al. 1982)
\ln \left( \frac{k_H}{MPa} \right) = 357.733 - \frac{19363.1}{(T/K)} - 9.04865 \cdot (T/K)^2 - 49.5296 \cdot \ln \left( \frac{T}{K} \right); \text{ maximum } k_H = 7.836 \times 10^4 \text{ MPa at } 372.1 \text{ K} \text{ (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* (27.9°C, EPICS-GC, measured range 27.9–45°C, Hansen et al. 1993)
\ln \left( \frac{[H]}{(kPa \cdot m^3/mol)} \right) = -8014/(T/K) + 30.0; \text{ temp range: } 27.9–45°C \text{ (EPICS-GC, Hansen et al. 1993)}
297951 (EPICS-GC, Ryu & Park 1999)
21838 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)
\log K_{AW} = 12.08 - 3263/(T/K) \text{ (summary of literature data, Staudinger & Roberts 2001)}
257797 (24.9°C, calculated-P/C, Sarrate et al. 2004)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

4.0 (calculated-π substituent const., Hansch et al. 1968; Hansch & Leo 1979)
5.29 (calculated-activity coefficient γ, 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 γ, Schantz & Martire 1987)
5.15 ± 0.45 (recommended, Sangster 1989; 1993)
5.61 (calculated-activity coefficients, Tse & Sandler 1994)
5.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.30 (calculated-measured γ∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):

Volatilization: \( t_{1/2} = 5.55 \) h for a water column of 1 m² minimum cross section of depth 1 m (Mackay & Leinonen 1975)
estimated \( t_{1/2} \sim 3.1 \) h at 20°C in a river 1 m deep flowing at 1 m s⁻¹ and with a wind velocity of 3 m s⁻¹ (Lyman et al. 1982).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O2} \) with O₂ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[
k_{OH}^{(exptl)} = 6.03 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, \quad k_{OH}^{(calc)} = 2.35 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K, measured range } 296–497 \text{ K (flash photolysis-kinetic spectroscopy, Greiner 1970)}
\]
\[
k_{O3(O3P)} = 1.70 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O(3P) atom at room temp. (Herron & Huie 1973)}
\]
\[
k_{O3(O3P)}^{(exptl)} = 8.42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K, } k_{OH}^{(calc)} = 7.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K (Darnall et al. 1978)}
\]
Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4–24$ h for $C_4H_{10}$ and higher paraffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction $k = 8.68 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with OH radicals with an estimated lifetime of 16 h in air during summer daylight (Altshuller 1991).

Surface water: volatilization $t_{1/2} = 5.55$ h for a water column of 1 m$^2$ minimum cross section of depth 1 m (Mackay & Leinonen 1975); estimated volatilization $t_{1/2} = 3.1$ h at 20°C in a river 1 m deep flowing at 1 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982).

Ground water:

Sediment:

Soil:

Biota:

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Pressures range from 0.0103 to 8.86 MPa

\[ \Delta H_{sol}/(kJ \text{ mol}^{-1}) = 13.3 \]

\[ \ln x = A + B/T + C \ln T \]

\[ T \text{ in K} \]

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FIGURE 2.1.1.23.1 Logarithm of mole fraction solubility (\( \ln x \)) versus reciprocal temperature for \( n \)-octane.
**TABLE 2.1.1.23.2**

Reported vapor pressures of \( n \)-octane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{C + T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a)
\]

\[
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\ln P = A - \frac{B}{C + T/K} \quad (2a)
\]

\[
\log P = A - \frac{B}{C + T/K} - C \log (T/K) \quad (3) \\
\ln \left(\frac{P/kPa}{P_0/kPa}\right) = [1 - (T_o/K)/(T/K)] \exp\{A_0 - A_1(T/K) + A_2(T/K)^2\} \quad (3a)
\]

\[
\ln \left(\frac{P/kPa}{P_0/kPa}\right) = [1 - (T_o/K)/(T/K)] \exp\{A_0 - A_1(T/K) + A_2(T/K)^2\} \quad (5) - Cox eq.
\]

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for temp 291–409 K
**TABLE 2.1.1.1.23.3**

Reported Henry's law constants and octanol-air partition coefficients of *n*-octane at various temperatures and temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \\
\ln (1/K_{AW}) &= A - B/(T/K) \\
\ln (k_{H}/\text{atm}) &= A - B/(T/K) \\
\ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) \\
K_{AW} &= A - B \cdot (T/K) + C \cdot (T/K)^2
\end{align*}
\]

Henry's law constant

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<td><strong>GC det'd activity coefficient</strong></td>
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* interpolated data
**FIGURE 2.1.1.123.3** Logarithm of Henry's law constant versus reciprocal temperature for \(n\)-octane.

**FIGURE 2.1.1.123.4** Logarithm of \(K_{OA}\) versus reciprocal temperature for \(n\)-octane.
2.1.1.24 4-Methyloctane

Common Name: 4-Methyloctane
Synonym:
Chemical Name: 4-methyloctane
CAS Registry No: 2216-34-4
Molecular Formula: C_{9}H_{20}; CH_{3}(CH_{2})_{2}CH(CH_{3})CH_{2}CH_{3}
Molecular Weight: 128.255
Melting Point (°C):
   -113.3 (Lide 2003)
Boiling Point (°C):
   142.4 (Lide 2003)
Density (g/cm³ at 20°C):
   0.7199, 0.7169 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
   178.2 (20°C, calculated-density)
   207.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
   44.75, 36.60 (25°C, normal bp, Dreisbach 1961)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
   0.115 (shake flask-GC, Price 1976; quoted, Shaw 1989)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
   901 (extrapolated-Antoine eq., Dreisbach 1959)
   log (P/mmHg) = 6.9155 – 1406.0/(206.0 + t°C); temp range 50–165°C (Antoine eq. for liquid state, Dreisbach 1959)
   933 (extrapolated-Antoine eq., temp range 32–170°C, Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.90318 – 1399.12/(205.41 + t°C); temp range 32–170°C (Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 11.2012 – 2.9467 × 10^{-3}/(T/K) + 1.2133·log (T/K) – 1.4423 × 10^{-4}·(T/K)^{2}; temp range 160–588 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°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 K_{ow}:
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{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, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{\text{OH}} = 9.72 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1989)
- $k_{\text{OH}} = 9.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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:** C₉H₂₀; CH₃(CH₂)₇CH₃  
**Molecular Weight:** 128.255  
**Melting Point (°C):**  
-53.46 (Lide 2003)  
**Boiling Point (°C):**  
150.82 (Lide 2003)  
**Density (g/cm³ at 20°C):**  
- 0.7176, 0.7138 (20°C, 25°C, Dreisbach 1959)  
- 0.7177, 0.7138 (20°C, 25°C, Riddick et al. 1986)  
**Molar Volume (cm³/mol):**  
- 178.7, 179.7 (20°C, 25°C, calculated-density)  
- 207.2 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, ΔHᵥ (kJ/mol):**  
- 44.442, 36.915 (25°C, bp, Riddick et al. 1986)  
- 46.55 (298.15 K, recommended, Ruzicka & Majer 1994)  
**Enthalpy of Fusion, ΔH₉ₚ₈ (kJ/mol):**  
- 15.468 (Dreisbach 1959; Riddick et al. 1986)  
- 6.28, 15.38 (–55.95, –53.45°C, Chickos et al. 1999)  
**Entropy of Fusion, ΔS₉ₚ₈ (J/mol K):**  
- 99.2, 100.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m³ or mg/L at 25°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°C, Price 1976)  
- 0.289, 0.272 (15, 20°C, 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°C, IUPAC Solubility Data Series, Shaw 1989)  
**In x = –433.434 + 18767.82/(T/K) + 61.940·ln (T/K); temp range 290–400 K (eq. derived from lit. calorimetric and solubility data, Tsonopoulos 1999)**  
- 0.135, 0.477 (25, 100.1°C, calculated-liquid-liquid equilibrium LLE data, Mączyński et al. 2004)  
**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):**  
- 6349* (70.127°C, ebulliometry, measured range 70.127–151.764°C, Willingham et al. 1945)  
**log (P/mmHg) = 6.94495 – 1435.158/(202.331 + t°C); temp range 70.1–151.8°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)**  
- 623* (70.343°C, ebulliometry-manometer, measured range 70.343–151.786°C, Forziati et al. 1949)  
**log (P/mmHg) = 6.93513 – 1428.811/(201.619 + t°C); temp range 70.343–151.786°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)**  
- 580 (extrapolated-Antoine eq., Dreisbach 1959)  
**log (P/mmHg) = 6.93513 – 1428.811/(201.619 + t°C); temp range 60–185°C (Antoine eq. for liquid state, Dreisbach 1959)**
Aliphatic and Cyclic Hydrocarbons

571* (extrapolated-Antoine eq., temp range 39.32–178.48°C, Zwolinski & Wilhoit 1971)

\[
\log (P/\text{mmHg}) = 6.93513 - 1428.811/(201.619 + t/°C); \text{ temp range 39.32–178.48°C (Antoine eq., Zwolinski & Wilhoit 1971)}
\]

570, 713 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.0628 – 1430.638/(201.827 + t/°C), temp range: 70.434–151.8°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

571 (extrapolated-Antoine eq., temp range 39–179°C, Dean 1985, 1992)

\[
\log (P/\text{mmHg}) = 6.93893 - 1431.82/(202.01 + t/°C); \text{ temp range 39–179°C (Antoine eq., Dean 1985, 1992)}
\]

570 (lit. average, Riddick et al. 1986)

\[
\log (P/\text{kPa}) = 6.06383 – 1431.82/(202.011 + t/°C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

517; 571 (extrapolated-Antoine eq.-I; interpolated -Antoine eq.-II, Stephenson & Malanowski 1987)

\[
\log (P/\text{kPa}) = 6.0593 – 1429.46/(-71.33 + T/K); \text{ temp range 344–426 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 8.17855 - 2523.8/(T/K); \text{ temp range 219–308 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

580.7* (recommended, Ruzicka & Majer 1994)

\[
\ln \left[ \frac{P/\text{kPa}}{(P_0/\text{kPa})} \right] = \left[ 1 - \left( \frac{T}{T_0} \right) \right] \cdot \exp \left[ 2.94690 - 2.061933 \times 10^{-3} \left( \frac{T}{T_0} \right) + 1.903683 \times 10^{-6} \left( \frac{T}{T_0} \right)^2 \right]; \text{ reference state at } P_0 = 101.325 \text{ kPa, } T_0 = 423.932 \text{ K (Cox equation, Ruzicka & Majer 1994)}
\]

41950* (EPICS-GC/FID, measured range 10–30ºC, Ashworth et al. 1988)

\[
\ln \left[ \frac{H/(\text{atm m}^3/\text{mol})}{(H_0/(\text{atm m}^3/\text{mol}))} \right] = -0.1847 + 202.1/(T/K); \text{ temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)}
\]

599600 (calculated-P/C, Eastcott et al. 1988)

459668 (EPICS-GC, Ryu & Park 1999)

42164 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

Octanol/Water Partition Coefficient, log \(K_{OW}\):

4.51 (estimated-HPLC-k′ correlation, Coates et al. 1985)

5.65 ± 0.60 (recommended, Sangster 1989)

5.42 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log \(K_{OA}\):

Bioconcentration Factor,

Sorption Partition Coefficient, log \(K_{OC}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):

Volutilization:

Photolysis:

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with \(NO_3\) radical and \(k_{O3}\) with \(O_3\) or as indicated, *data at other temperatures see reference:
$k_{OH} = (10.7 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \pm 2 \text{ K (relative rate method, Atkinson et al. 1982a, 1984c)}$

$k_{OH} = 10.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 312 \text{ K in smog chamber (Nolting et al. 1988)}$

$k_{OH} = 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)}$

$k_{OH} = 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, } k_{NO_3} = 2.39 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (Atkinson 1990)}$

$k_{OH} = 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ estimated atmospheric lifetime of } 14 \text{ h (Altshuller 1991)}$

$k_{OH} = 1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K, } k_{NO_3} = 2.30 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Sabljic & Güsten 1990)}$

$k_{NO_3} = 2.41 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (Atkinson 1991)}$

$k_{NO_3}(\text{exptl}) = (1.92, 2.59) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3}(\text{calc}) = 2.47 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \pm 2 \text{ K (relative rate method, Aschmann & Atkinson 1995)}$

$k_{OH}^{*} = 10.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 2.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)}$

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_\text{a} \sim 2.4–24 \text{ h for } C_4H_{10} \text{ and higher paraffins for the reaction with hydroxyl radical, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976); photooxidation reaction rate constant of } 1.02 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with OH radical with an estimated lifetime } t = 14 \text{ h during summer daylight (Altshuller 1991)}$.

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<th>Temperature (°C)</th>
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<th>Jonsson et al. 1982</th>
<th>Shaw 1989a</th>
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FIGURE 2.1.1.25.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for $n$-nonane.

TABLE 2.1.1.25.2
Reported vapor pressures of $n$-nonane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \log (T/K) \quad (4) \\
\ln \left[ \frac{(P/kPa)/(P_0/kPa)}{1 - \frac{T_0/K}{T/K}} \right] &= \exp \left[ A_0 - A_1 \frac{T/K}{T/K} + A_2 \left( T/K \right)^2 \right] \quad (5) - \text{Cox eq.}
\end{align*}
\]

1.

<table>
<thead>
<tr>
<th>Willingham et al. 1945</th>
<th>Stull 1947</th>
<th>Forziati et al. 1949</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
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<td><strong>ebulliometry-manometer</strong></td>
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<td><strong>ebulliometry-manometer</strong></td>
<td><strong>selected values</strong></td>
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<td>$t/°C$</td>
<td>$P/Pa$</td>
<td>$t/°C$</td>
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## TABLE 2.1.1.25.2 (Continued)

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<td>ebulliometry-manometer</td>
<td>selected values</td>
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<td>( P/\text{Pa} )</td>
<td>( t/\degree C )</td>
<td>( P/\text{Pa} )</td>
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<td>( C )</td>
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<td>temp range: 70.1–151.8\degree C</td>
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### 2.

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<td>( A_2 )</td>
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Aliphatic and Cyclic Hydrocarbons

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 \( n \)-nonane at various temperatures and temperature dependence equations**

\[
\begin{align*}
\ln K_{\text{AW}} &= A - B/(T/K) \quad (1) \\
\log K_{\text{AW}} &= A - B/(T/K) \quad (1a) \\
\ln (1/K_{\text{AW}}) &= A - B/(T/K) \quad (2) \\
\log (1/K_{\text{AW}}) &= A - B/(T/K) \quad (2a) \\
\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] &= A - B/(T/K) \quad (3a) \\
\log [H/(\text{atm} \cdot \text{m}^3/\text{mol})] &= A - B/(T/K) \quad (3) \\
K_{\text{AW}} &= A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Jönsson et al. 1982</th>
<th>Ashworth et al. 1988</th>
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<tbody>
<tr>
<td>( t/°C )</td>
<td>( H/(\text{Pa} \cdot \text{m}^3/\text{mol}) )</td>
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\[ A = -0.1847 \]
\[ B = 202.1 \]

**Experimental data**

- Jönsson et al. 1982
- Žwolinski & Wilhoit 1971
- Ruzicka & Majer 1994

**b.p.** = 150.82 °C
**m.p.** = -53.46 °C
FIGURE 2.1.1.25.3 Logarithm of Henry's law constant versus reciprocal temperature for \( n \)-nonane.
### n-Decane

**Common Name:** n-Decane  
**Synonym:** decane  
**Chemical Name:** n-decane  
**CAS Registry No:** 124-18-5  
**Molecular Formula:** C\(_{10}\)H\(_{22}\); CH\(_3\)(CH\(_2\))\(_8\)CH\(_3\)  
**Molecular Weight:** 142.282

**Melting Point (°C):**  
-29.6  (Lide 2003)

**Boiling Point (°C):**  
174.15  (Lide 2003)

**Density (g/cm\(^3\) at 20°C):**  
0.7301, 0.7273 (20°C, 25°C, Dreisbach 1959)  
0.7301, 0.7264 (20°C, 25°C, Riddick et al. 1986)

**Molar Volume (cm\(^3\)/mol):**  
194.9, 195.9 (20°C, 25°C, calculated-density)  
229.4  (calculated-Le Bas method at normal boiling point)

**Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):**  
51.42  (209.15 K, recommended, Ruzicka & Majer 1994)

**Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):**  
28.72  (Dreisbach 1959)  
28.677  (Riddick et al. 1986)  
28.7  (Chickos et al. 1999)

**Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):**  

**Fugacity Ratio at 25°C, F:** 1.0

**Water Solubility (g/m\(^3\) or mg/L at 25°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, Krasnoshechekova & 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  (20°C, 25°C, tentative best values, IUPAC Solubility Data Series, Shaw 1989)  
0.0277, 0.0261  (20°C, 25°C, calculated-recommended liquid-liquid equilibrium LLE data, temp range 273.2–422.7 K, Mączyński et al. 2004)

**Vapor Pressure (Pa at 25°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*  (8.50°C, static-McLeod gauge, measured range –3.80 to 8.50°C, Linder 1931)  
7649*  (94.481°C, ebulliometry, measured range 94.481–175.121°C, Willingham et al. 1945)  
\[\log (P/mmHg) = 6.95367 – 1501.268/(194.480 + t°C); \text{ temp range } 94.6–175.1°C (\text{Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945})\]  
238*  (calculated-Antoine eq. regression, temp range 17.1–173°C, Stull 1947)  
182  (extrapolated-Antoine eq., Dreisbach 1959)  
\[\log (P/mmHg) = 6.95367 – 1501.268/(194.480 + t°C); \text{ temp range } 75–210°C (\text{Antoine eq. for liquid state, Dreisbach 1959})\]  
180*  (extrapolated-Antoine eq., temp range 57.7–202.9°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.95367 – 1501.268/(194.480 + t/°C); temp range 57.7–202.9°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = –0.2185 × 10^{912.0/(T/K)} + 8.248089; temp range 17.1–173°C (Antoine eq., Weast 1972–73)

86.53* (16.74°C, gas saturation, measured range –29.65 to 37.45°C, Carruth & Kobayashi 1973)

174 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.08321 – 1504.405/(194.831 + t/°C); temp range 94.48–175.1°C (Antoine eq. from reported exper. data, Boublik et al. 1984)

log (P/kPa) = 6.94365 – 1495.17/(193.86 + t/°C); temp range 58–203°C (Antoine eq., Dean 1985, 1992)

173 (extrapolated-Antoine eq., temp range 58–203°C, Dean 1985, 1992)

log (P/kPa) = 5.55216 – 1594.49/(126.36 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

171 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 6.80914 – 1900.343/(–47.319 + T/K); temp range 252–383 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 5.069206 – 150.415/(–77.646 + T/K); temp range 373–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.04899 – 1482.502/(–80.635 + T/K); temp range 447–526 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 9.71412 – 6858.314/(454.63 + T/K); temp range 524–617 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

874.1* (50.64°C, static-quartz pressure gauge, measured range 50.64–314.982°C, Morgan & Kobayashi 1994)

182* (recommended, Ruzicka & Majer 1994)

ln [(P/kPa)/(P_0/kPa)] = [1 – (T_0/K)/(T/K)]·exp{2.96690 – 1.932579 × 10^{-3}·(T/K) + 1.644626 × 10^{-6}·(T/K)^2}; reference state at P_0 = 101.325 kPa, T_0 = 447.269 K (Cox equation, Ruzicka & Majer 1994)

log (P/mmHg) = 26.5125 – 3.3584 × 10^{3/(T/K)} – 6.1174·log (T/K) – 3.3225 × 10^{–10}·(T/K) + 4.8554 × 10^{–7}·(T/K)^2; temp range 243–618 K (vapor pressure eq., Yaws 1994)

127.6* (20°C, ebulliometer and inclined piston gauge, measured temp range 268–490 K. Chirico et al. 1989)

324 (liquid P_L, GC-RT correlation; Donovan 1996)

520* (41.6°C, ebulliometry, measured range 314.75–458.45 K, Dejoz et al. 1996)

ln (P/kPa) = 13.9735 – 3441.40/[(T/K) – 79.434]; temp range 314.75–458.45 K (ebulliometry, Dejoz et al. 1996)

Henry’s Law Constant (Pa m^3/mol at 25°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 K_{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 ± 0.70 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{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, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ as indicated, *data at other temperatures see reference:

$v_{\text{OH}} = (11.4 \pm 0.6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 299 \pm 2 K (relative rate method, Atkinson et al. 1982a, 1984c)

$v_{\text{OH}} = 11.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 312 K in a smog chamber (Nolting et al. 1988)

$v_{\text{OH}} = 1.16 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990, 1991)

$v_{\text{OH}} = 11.6 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, atmospheric lifetime of 12 h during summer daylight (Altshuller 1991)

$v_{\text{NO}_3}(\text{exptl}) = 2.59 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $v_{\text{NO}_3}(\text{calc}) = 2.47 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 \pm K (relative rate method, Aschmann & Atkinson 1995)

$v_{\text{OH}*} = 11.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $v_{\text{NO}_3} = 2.8 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4$–24 h for C$_4$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 $k = 1.16 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with hydroxyl radical with an estimated lifetime of 12 h during summer daylight (Altshuller 1991).

**TABLE 2.1.1.26.1**

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

$log P = A - B/(T/K) \quad (1)$

$log P = A - B/(C + t/°C) \quad (2)$

$log P = A - B/(C + T/K) \quad (3)$

$log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$

$log (P/P_{ref}) = [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2) \quad (5)$

1. **Linder 1931**

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2. **Willingham et al. 1945**

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4. **Zwolinski & Wilhoit 1971**

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(C)ontinued
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### 2.

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Data fitted to Wagner eq.

**FIGURE 2.1.1.26.1** 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: C\textsubscript{11}H\textsubscript{24}; CH\textsubscript{3}(CH\textsubscript{2})\textsubscript{9}CH\textsubscript{3}
Molecular Weight: 156.309
Melting Point (°C): –25.5 (Lide 2003)
Boiling Point (°C): 195.9 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
\begin{itemize}
  \item 0.74024, 0.73652 (20°C, 25°C, Camin & Rossini 1955)
  \item 0.7402, 0.7366 (20°C, 25°C, Dreisbach 1959)
\end{itemize}
Molar Volume (cm\textsuperscript{3}/mol):
\begin{itemize}
  \item 211.2 (20°C, calculated-density)
  \item 251.6 (calculated-Le Bas method at normal boiling point)
\end{itemize}
Enthalpy of Vaporization, Δ\textsubscript{HV} (kJ/mol): 56.5, 41.524 (25°C, bp, Dreisbach 1959)
Enthalpy of Fusion, Δ\textsubscript{Hfus} (kJ/mol): 6.86, 22.18, 29.03 (–36.55, –25.55°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, Δ\textsubscript{Sfus} (J/mol K): 118.6, 119.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
\begin{itemize}
  \item 0.0044 (shake flask-GC, McAuliffe 1969)
  \item 0.0036 (shake flask-GC, Krashoshchekova & Gubertritis 1973)
  \item 0.0040 (“best” value, IUPAC Solubility Data Series, Shaw 1989)
  \item 0.0042 (calculated-recommended liquid-liquid equilibrium LLE data, Mączyński et al. 2004)
\end{itemize}
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
\begin{itemize}
  \item 133.3* (31.4°C, summary of literature data, temp range 31.4–194.5°C, Stull 1947)
  \item \log (P/mmHg) = 6.97674 – 1572.477/(188.022 + t/°C); temp range 105.4–197.3°C (Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)
  \item 57.18 (extrapolated-Antoine eq., Dreisbach 1959)
  \item \log (P/mmHg) = 6.97674 – 1572.477/(188.022 + t/°C); temp range 98–258°C (Antoine eq. for liquid state, Dreisbach 1959)
  \item 52.20* (extrapolated-Antoine eq., temp range 75.1–225.8°C, Zwolinski & Wilhoit 1971)
  \item \log (P/mmHg) = 6.97220 – 1569.57/(187.700 + t/°C); temp range 75.1–225.8°C (Antoine eq., Zwolinski & Wilhoit 1971)
  \item \log (P/mmHg) = –0.2185 × 11481.7/(T/K) + 8.260477; temp range 31.4–194.5°C (Antoine eq., Weast 1972–73)
  \item 52.5 (extrapolated-Antoine eq., Boublik et al. 1984)
  \item \log (P/kPa) = 6.12013 – 1572.031/(188.062 + t/°C); temp range 104.5–197.3°C (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)
  \item \log (P/mmHg) = 6.97220 – 1569.57/(187.70 + t/°C); temp range 75–226°C (Antoine eq., Dean 1985, 1992)
  \item 54.8 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
  \item \log (P/kPa) = 6.10154 – 1572.411/(–85.128 + T/K); temp range 278–470 K (Antoine eq., Stephenson & Malanowski 1987)
  \item 56.89* (recommended, Ruzicka & Majer 1994)
\end{itemize}
ln [(P/kPa)/(P_0/kPa)] = [1 – (T/K)/(T_0/K)]·exp{3.02771 – 2.045579 × 10^{-3}(T/K) + 1.712658 × 10^{-6}(T/K)^2}; reference state at P_0 = 101.325 kPa, T_0 = 469.042 K (Cox equation, Ruzicka & Majer 1994)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 82.9230 - 5.6085 \times 10^3/(T/K) - 23.7327 \cdot \log (T/K) + 1.0469 \times 10^{-2} \cdot (T/K) + 7.087 \times 10^{-13} \cdot (T/K)^2; \text{ temp range 248–639 K (vapor pressure eq., Yaws 1994)} \]

Henry’s Law Constant (Pa m^3/mol at 25°C):
- 185000 \quad \text{(calculated-P/C, Mackay & Shiu 1981)}
- 185390 \quad \text{(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)}

Octanol/Water Partition Coefficient, log K_{ow}:
- 6.94 \quad \text{(estimated-HPLC/MS, Burkhard et al. 1985)}
- 6.51 \quad \text{(calculated-fragment const., Burkhard et al. 1985)}

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Vaporization:

Photolysis:

Oxidation: rate constant k for gas-phase second order rate constants, k_{oh} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
- k_{oh} = 13.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 312 K in a smog chamber (Nolting et al. 1988)
- k_{oh} = 1.32 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 298 K (recommended, Atkinson 1989, 1990)
- k_{oh} = 1.29 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

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\[ \Delta H_v/(kJ \text{ mol}^{-1}) = \]

at 25°C 56.34
at bp 41.50

FIGURE 2.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for \( n \)-undecane.
2.1.1.1.28  n-Dodecane

Common Name: n-Dodecane
Synonym: dodecane
Chemical Name: n-dodecane
CAS Registry No: 112-40-3
Molecular Formula: C_{12}H_{26}; CH_{3}(CH_{2})_{10}CH_{3}
Molecular Weight: 170.334
Melting Point (°C):
-9.57  (Lide 2003)
Boiling Point (°C):
216.32  (Lide 2003)
Density (g/cm³ at 20°C):
0.7487, 0.7452  (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
0.74941  (20°C, densimeter, Dejoz et al. 1996)
Molar Volume (cm³/mol):
227.5  (20°C, calculated-density, Stephenson & Malanowski 1987)
273.8  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
61.287, 43.64  (25°, bp, Riddick et al. 1986)
61.52  (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
36.84  (Dreisbach 1959)
35.86  (Riddick et al. 1986)
36.82  (Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
139.75, 128.5  (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F:
1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°C or as indicated and reported temperature dependence equations. Additional data at other
temperatures designated * are compiled at the end of this section.):
6365*  (126.31°C, ebulliometry, measured range 126.31–217.345°C, Willingham et al. 1945)
log (P/mmHg) = 6.98059 – 1625.928/(180.311 + t/°C); temp range 126.4–217.3°C (Antoine eq. from exptl. data,
ebuliometry-manometer, Willingham et al. 1945)
133.3*  (47.7°C, summary of literature data, temp range 47.7–214.5°C, Stull 1947)
17.60  (extrapolated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.98059 – 1625.928/(180.311 + t/°C); temp range 150–280°C (Antoine eq. for liquid state,
Dreisbach 1959)
15.70*  (extrapolated-Antoine eq., temp range 91.47–247.08°C, Zwolinski & Wilhoit 1971)
7.60  (derived from compiled data, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.99795 – 1639.27/(181.835 + t/°C); temp range 91.47–247.08°C (Antoine eq., Zwolinski &
Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 11857.7/(T/K)] + 8.150997; temp range 47.7–345.8°C (Antoine eq., Weast 1972–73)
15.5  (Antoine eq., Boublik et al. 1973, 1984)
log (P/mmHg) = 6.9829 – 1627.714/(180.521 + t/°C); temp range 104.5–197.3°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 (P/kPa) = 6.1074 – 1627.417/(180.489 + t°C); temp range 104.5–197.3°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)
log (P/mmHg) = 6.99795 – 1639.27/(181.84 + t°C); temp range 91–247°C (Antoine eq., Dean 1985, 1992)

17.3* (24.931°C, gas saturation, measured temp range 298.081–389.66 K, Allemand et al. 1986)
16.0 (lit. average, Riddick et al. 1986)
log (P/kPa) = 6.12285 – 1639.27/(181.835 + t/K); temp range not specified (Antoine eq., Riddick et al. 1986)

18.6 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.62064 – 1942.122/(–65.587 + T/K); temp range 278–400 K (Antoine eq.-I, Stephenson & Malanowski 1987)


Henry’s Law Constant (Pa m3/mol at 25°C):
723000 (calculated-P/C, Bobra et al. 1979)

822000, 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 KOW:
7.24, 7.04 (estimated-HPLC/MS, calculated-fragment const., Burkhard et al. 1985)
6.10 (Coates et al. 1985)
6.60 ± 1.00 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log KOA:

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constant, k, and Half-Lives, t½:
Volatilization: rate constants: k = 0.60 d⁻¹, t½ = 1.1 d in spring at 8–16°C, k = 0.97 d⁻¹, t½ = 0.7 d in summer at 20–22°C, k = 0.20 d⁻¹, t½ = 3.6 d in winter at 3–7°C for the periods when volatilization appears to dominate, and k = 0.377 d⁻¹, t½ = 1.8 d with HgCl₂, and k = 1.085 d⁻¹, t½ = 0.64 d without HgCl₂ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, kOH for reaction with OH radical, kNO₃ with NO₃ radical and kO₃ with O₃ as indicated, *data at other temperatures see reference:
kOH = 15.1 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 312 K in a smog chamber (Nolting et al. 1988)
kOH = 14.2 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990)
kOH = 13.9 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:
Half-Lives in the Environment:

Air: Surface water: estimated $t_{1/2} = 0.5$ d for surface waters in case of first order reduction process (Zoeteman et al. 1980)

marine mesocosm $t_{1/2} = 1.1$ d at 8–16°C in spring, $t_{1/2} = 0.7$ d at 20–22°C in summer and $t_{1/2} = 3.6$ h at 3–7°C in winter when volatilization dominates, and $t_{1/2} = 1.8$ d with HgCl$_2$ as poison, and $k = 1.085$ d$^{-1}$, $t_{1/2} = 0.64$ d without poison in mid-September (Wakeham et al. 1983)

### TABLE 2.1.1.1.28.1

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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\ln P &= A - B/(C + T/K) \quad (3a) \\
\log P &= A - B/(T/K) - C\log (T/K) \quad (4) \\
\ln P &= A - B/(T/K) \quad (4a) \\
\ln (P/P_{ref}) &= [1 - (T_{ref}/T)]\exp(a + bT + cT^2) \quad (5) - Cox eq.
\end{align*}
\]

1. \textbf{Willingham et al. 1945} \textit{ebulliometry} \hspace{1cm} \textbf{Stull 1947} \textit{summary of literature data} \hspace{1cm} \textbf{Zwolinski & Wilhoit 1971} \textit{selected values} \hspace{1cm} \textbf{Allemand et al. 1986} \textit{gas saturation}

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| C | 180.311 | C | 181.835 | \( \Delta H_v/(kJ \text{ mol}^{-1}) = \)
| | | at 25°C | 61.59 | at bp | 43.64 |

(Continued)
### TABLE 2.1.1.28.1 (Continued)

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FIGURE 2.1.1.28.1 Logarithm of vapor pressure versus reciprocal temperature for $n$-dodecane.
2.1.1.29  n-Tridecane

Common Name: Tridecane
Synonym:  
Chemical Name: \( n \)-tridecane  
CAS Registry No: 629-50-5  
Molecular Formula: \( \text{C}_{13}\text{H}_{28} \); \( \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \)  
Molecular Weight: 184.361  
Melting Point (°C):
  - 5.4 (Lide 2003)
Boiling Point (°C):
  235.47 (Lide 2003)
Density (g/cm³):
  0.76522, 0.75270 (20°C, 25°C, Camin & Rossini 1955)
  0.7564, 0.7528 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
  296.0 (calculated-Le Bas method at normal boiling point)
  243.7 (20°C, Stephenson & Malanowski 1987)
Enthalpy of Vaporization, \( \Delta_{HV} \) (kJ/mol):
  66.23, 45.65 (25°C, bp, Riddick et al. 1986)
  66.68 (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, \( \Delta_{Hfus} \) (kJ/mol):
  28.501 (Riddick et al. 1986)
  7.66, 28.49; 36.15 (–18.15, –5.35°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, \( \Delta_{Sfus} \) (J/mol K):
  136.31, 137.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  0.00104 (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
  0.0047–0.0217 (estimated, Coates et al. 1985)
  0.06 (Riddick et al. 1986)
  0.33; 0.198 (measured; calculated molar volume correlation, Wang et al. 1992)
Vapor Pressure (Pa at 25°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* (59.4°C, summary of literature data, temp range 59.4–234.0°C, Stull 1947)
  5530* (139.3°C, ebulliometry, measured range 139.3–236.065°C, Camin & Rossini 1955)
  \( \log (P/\text{mmHg}) = 7.00339 – 1689.093/ (174.284 + t/°C) \); temp range 145.1–236.1°C (Antoine eq., ebulliometry-manometer measurements; Camin & Rossini 1955)
  5.30 (extrapolated-Antoine eq., Dreisbach 1959; quoted, Riddick et al. 1986)
  \( \log (P/\text{mmHg}) = 6.9887 – 1677.43/(172.90 + t/°C) \); temp range 131–302°C (Antoine eq. for liquid state, Dreisbach 1959)
  5.73* (derived from compiled data, Zwolinski & Wilhoit 1971)
  \( \log (P/\text{mmHg}) = 7.00756 – 1690.67/(107.20 + t/°C) \); temp range 107.2–267.04°C (Antoine eq., Zwolinski & Wilhoit 1971)
  \( \log (P/\text{mmHg}) = [–0.2185 × 12991.3/(T/K)] + 8.481732; \) temp range 59.4–234°C (Antoine eq., Weast 197–73)
  \( \log (P/\text{mmHg}) = 7.00925 – 1693.684/(t/°C + 174.815); \) temp range 139–236°C (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublík et al. 1973)
  \( \log (P/\text{kPa}) = 6.13542 – 1694.624/(t/°C + 174.916); \) temp. range 139–236°C (Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublík et al. 1984)
  \( \log (P/\text{mmHg}) = 7.00756 – 1690.67/(174.22 + t/°C); \) temp range 107–267°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 6.13246 – 1690.67/(174.220 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/mmHg) = 7.00756 – 1690.67/(t/°C + 174.22); temp range 107–267°C, (Antoine eq., Dean 1985; 1992)
log (P/kPa) = 6.13546 – 1690.67/(T/K – 98.93); temp range 417–511 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

5.682* (recommended, Ruzicka & Majer 1994)

\[ \log \left( \frac{P}{kPa} \right) = \frac{A - B}{C + T/K} \] (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol at 25°C):
233351 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, \( \log K_{ow} \):
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, \( \log K_{oa} \):

Bioconcentration Factor, \( \log BCF \) or \( \log K_b \):

Sorption Partition Coefficient, \( \log K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation:
rate constant \( k \) for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with
NO₃ radical and \( k_{O_3} \) with O₃ or as indicated, *data at other temperatures see reference:

\[ k_{OH} = 17.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 312 \text{ K in a smog chamber (Nolting et al. 1988)} \]

\[ k_{OH} = 15.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K, } 17.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 302 \text{ K (Atkinson 1989)} \]

\[ k_{OH} = 16.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989, 1990, 1997)} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:

### TABLE 2.1.1.1.29.1

Reported vapor pressures of \( n \)-tridecane at various temperatures and the coefficients for the vapor pressure equations

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**FIGURE 2.1.1.29.1** Logarithm of vapor pressure versus reciprocal temperature for n-tridecane.
2.1.1.30  n-Tetradecane

Common Name: Tetradecane
Synonym:
Chemical Name: \( n \)-tetradecane
CAS Registry No: 629-59-4
Molecular Formula: \( C_{14}H_{30} \); \( CH_3(CH_2)_{12}CH_3 \)
Molecular Weight: 198.388
Melting Point (°C):
5.82 (Lide 2003)
Boiling Point (°C):
253.58 (Lide 2003)
Density (g/cm³):
0.76275, 0.75917 (20°C, 25°C, Camin & Rossini 1955)
0.7628, 0.7593 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
260.1 (20°C, Stephenson & Malanowski 1987)
318.2 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
71.13, 47.73 (25°C, bp, Dreisbach 1961)
71.73 (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
45.07 (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
161.54, 147.1 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
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°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* (76.4°C, summary of literature data, temp range 76.4–252.5°C, Stull 1947)
\[
\log (P/mmHg) = 7.01245 - 1739.623/(167.534 + t/°C); \text{ temp range } 165.9–254.2°C \quad \text{(Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)}
\]
1.56 (extrapolated-Antoine eq., Dreisbach 1959)
\[
\log (P/mmHg) = 6.9957 - 1725.46/(165.75 + t/°C); \text{ temp range } 147–325°C \quad \text{(Antoine eq. for liquid state, Dreisbach 1959)}
\]
1.27* (Antoine eq., temp range 121.80–286.0°C, Zwolinski & Wilhoit 1971)
1.867 (derived from compiled data, Zwolinski & Wilhoit 1971)
\[
\log (P/mmHg) = 7.01300 - 1740.88/(167.720 + t/°C); \text{ temp range } 121.80–286.0°C \quad \text{(Antoine eq., Zwolsinksi & Wilhoit 1971)}
\]
\[
\log (P/mmHg) = [-0.2185 \times 13750.0/(T/K)] + 8.628699; \text{ temp range } 76.4–252.5°C \quad \text{(Antoine eq., Weast 1972–73)}
\]
1.30 (extrapolated-Antoine eq., Boublík et al. 1973, 1984)
\[
\log (P/mmHg) = 7.02216 - 1747.452/(t/°C + 168.437); \text{ temp range } 155–254°C \quad \text{(Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublík et al. 1973)}
\]
\[
\log (P/kPa) = 6.14914 - 1749.052/(t/°C + 168.611); \text{ temp range } 155–254°C \quad \text{(Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublík et al. 1984)}
\]
log \( \log(P/\text{mmHg}) = 7.01300 - 1740.88/(T/\degree\text{C} + 167.72); \) temp. range 112–286°C (Antoine eq., Dean 1985; 1992)
72.0* (70.01°C, gas saturation, measured temp range 343.16–394.73 K, Allemand et al. 1986)
log \( \log(P_t/\text{kPa}) = 6.62828 - 2063.84/(T/K - 77.378); \) temp range 313–433 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
log \( \log(P_t/\text{kPa}) = 6.1379 - 1740.88/(T/K - 105.43); \) temp. range 432–529 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
1.804* (recommended, Ruzicka & Majer 1994)
ln \( \ln[(P/\text{kPa})/(P^o/\text{kPa})] = [1 - (T_o/K)/(T/K)] \cdot \exp{3.13624 - 2.063853 \times 10^{-3} \cdot (T/K) + 1.541507 \times 10^{-6} \cdot (T/K)^2}; \) reference state at \( P^o = 101.325 \text{kPa}, T_o = 526.691 \text{K} \) (Cox equation, Ruzicka & Majer 1994)
log \( \log(P/\text{mmHg}) = 106.1056 - 7.3461 \times 10^3/(T/K) - 31.5195 \cdot \log(T/K) + 1.2356 \times 10^{-2} \cdot (T/K) - 8.3955 \times 10^{-13} \cdot (T/K)^2; \) temp range 279–692 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°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 \( K_{ow}: \)
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 \( K_{oa}: \)
Bioconcentration Factor, log \( BCF \) or log \( K_b: \)

Sorption Partition Coefficient, log \( K_{oc}: \)

Environmental Fate Rate Constants, \( k, \) and Half-Lives, \( t_\frac{1}{2}: \)
Volatilization:
Photolysis:
Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO3}} \) with NO₃ radical and \( k_{\text{O3}} \) with O₃ or as indicated, *data at other temperatures see reference:
\( k_{\text{OH}} = 19.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 312 K in a smog chamber (Nolting et al. 1988)
\( k_{\text{OH}} = 19.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 312 K (Atkinson 1989)
\( k_{\text{OH}} = 19.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Atkinson 1990)
\( k_{\text{OH}} = 18.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation: microbial degradation \( t_\frac{1}{2} \leq 15 \text{ d} \) by \textit{Pseudomonas sp.} (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants \( k_1 \) and \( k_2): \)
Half-Lives in the Environment:
TABLE 2.1.1.30.1
Reported vapor pressures of *n*-tetradecane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(T/K) + C \cdot \log (T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\ln (P/P_{ref}) &= [1 - (T_{ref}/T)] \cdot \exp(a + bT + cT^2) \quad (5) \text{- Cox eq.}
\end{align*}
\]

1. Stull 1947

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<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
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(Continued)
TABLE 2.1.1.30.1 (Continued)

2.

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Data fitted to Wagner eq.

FIGURE 2.1.1.30.1 Logarithm of vapor pressure versus reciprocal temperature for n-tetradecane.
### n-Pentadecane

**Common Name:** Pentadecane  
**Synonym:**  
**Chemical Name:** \( n \)-pentadecane  
**CAS Registry No:** 629-62-9  
**Molecular Formula:** \( C_{15}H_{32} \); \( CH_3(CH_2)_{13}CH_3 \)  
**Molecular Weight:** 212.415  
**Melting Point (°C):**  
9.95 (Lide 2003)  
**Boiling Point (°C):** 270.6 (Camin & Rossini 1955; Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)  
**Density (g/cm³):**  
0.76830, 0.76488 (20°C, 25°C, Camin & Rossini 1955)  
0.7685, 0.7650 (20°C, 25°C, Dreisbach 1959)  
**Molar Volume (cm³/mol):**  
276.4 (20°C, calculated-density)  
340.4 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):**  
76.16, 49.41 (25°C, bp, Dreisbach 1961)  
76.77 (298.15 K, recommended, Ruzicka & Majer 1994)  
**Enthalpy of Fusion, \( \Delta H_{ fus} \) (kJ/mol):**  
9.17, 34.6; 43.77 (–2.25, 9.95; total phase change enthalpy, Chickos et al. 1999)  
**Entropy of Fusion, \( \Delta S_{ fus} \) (J/mol K):**  
156.02, 156.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m³ or mg/L at 25°C):**  
7.6 × 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°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* (91.6°C, summary of literature data, temp range 91.6–270.5°C, Stull 1947)  
\( \log (P/mmHg) = 7.02445 − 1789.658/(161.291 + t/°C) \); temp range 169.6–270.6°C (Antoine eq., ebulliometry-manometer measurements, Camin & Rossini 1955)  
0.311 (extrapolated-Antoine eq., Dreisbach 1959)  
\( \log (P/mmHg) = 7.0017 − 1768.82/(158.60 + t°C) \); temp range 160–338°C (Antoine eq. for liquid state, Dreisbach 1959)  
1333* (135.8°C, derived from compiled data, temp range 135.8–270.685°C, Zwolinski & Wilhoit 1971)  
\( \log (P/mmHg) = 7.01359 − 1789.95/(161.380 + t°C) \); temp range 135.8–303.8°C (Antoine eq., Zwolinski & Wilhoit 1971)  
\( \log (P/mmHg) = [−0.2185 × 14635.9/(T/K)] + 8.822087; \) temp range 91.6–270.5°C (Antoine eq., Weast 1972–73)  
0.356 (extrapolated-Antoine eq., Boublik et al. 1973)  
\( \log P/mmHg = 7.03121 − 1797.239/(t°C + 164.128); \) temp range 170–270°C (Antoine eq. from exptl. data of Camin & Rossini 1955, Boublik et al. 1973)  
0.359 (extrapolated-Antoine eq., Boublik et al. 1984)  
\( \log (P/kPa) = 6.15888 − 1797.239/(t°C + 162.128); \) temp range 170–270.5°C (Antoine eq. derived from exptl. data of Camin & Rossini 1955, Boublik et al. 1984)  
\( \log (P/mmHg) = 7.02359 − 1789.95/(161.38 + t°C); \) temp range 136–304°C (Antoine eq., Dean 1985, 1992)  
15.87* (60.0°C, gas saturation, measured temp range 60.0–136.0°C, Allemand et al. 1986)

log \( (P_l/kPa) = 6.14849 - 1789.95/(T/K - 111.77) \); temp range 447–546 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

0.576* (recommended, Ruzicka & Majer 1994)

\[ \ln \left( \frac{(P/kPa)/(P_o/kPa)} \right) = \left[ 1 - \frac{(T_o/K)}{(T/K)} \right] \times \exp \{3.16144 - 2.062348 \times 10^{-3} \times (T/K) + 1.487263 \times 10^{-6} \times (T/K)^2 \}; \]

reference state at \( P_o = 101.325 \) kPa, \( T_o = 543.797 \) K (Cox equation, Ruzicka & Majer 1994)

\[ \log (P/mmHg) = 116.5157 - 8.041 \times 10^{3}/(T/K) - 38.799 \times \log (T/K) - 1.3398 \times 10^{-2} \times (T/K) - 4.4444 \times 10^{-6} \times (T/K)^2; \]

temp range 283–707 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa·m^3/mol at 25°C):

48535 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

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, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \) or \( \log K_{b} \):

Sorption Partition Coefficient, \( \log K_{OC} \):

Environmental Fate Rate Constant, \( k \), and Half-Lives, \( t_{1/2} \):

Vaporization: vaporization rate constant of \( k = 0.69 \) d\(^{-1}\) with a water column \( t_{1/2} = 1.0 \) d at 6–18°C, in spring; \( k = 0.85 \) d\(^{-1}\) with a water column \( t_{1/2} = 0.8 \) d at 20–22°C in summer; \( k = 0.16 \) d\(^{-1}\) with a water column \( t_{1/2} = 4.3 \) d at 3–7°C in winter for mesocosm experiment in coastal marine environment when volatilization dominates, volatilization \( k = 0.343 \) d\(^{-1}\) with a water column \( t_{1/2} = 2.0 \) d with HgCl\(_2\) poisoned water tank and \( k = 1.241 \) d\(^{-1}\) with a water column \( t_{1/2} = 0.56 \) 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, \( k_{OH} \) for reaction with OH radical, \( k_{O3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) as indicated, *data at other temperatures see reference:

\[ k_{OH} = 22.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 312 \text{ K in a smog chamber (Nolting et al. 1988)} \]

\[ k_{OH} = 22.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 312 \text{ K (Atkinson 1989)} \]

\[ k_{OH} = 22.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1990)} \]

\[ k_{OH} = 22.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (experimental); } 17.87 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Atmospheric Oxidation Program); and } 7.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Fate of Atmospheric Pollutants) for gas-phase reaction with OH radicals (Meylan & Howard 1993)} \]

\[ k_{OH} = 21.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)} \]

Hydrolysis:

Biodegradation: microbial degradation \( t_{1/2} < 15 \) d by *Pseudomonas sp.* (Setti et al. 1993)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:

Surface water: water column half-lives, \( t_{1/2} = 1.0 \) d, 6–18°C, in spring; \( t_{1/2} = 0.8 \) d, 20–22°C, in summer; \( t_{1/2} = 4.3 \) d, 3–7°C, in winter for mesocosm experiment in coastal marine mesocosm; \( t_{1/2} = 2.0 \) d with HgCl\(_2\) poisoned water tank and \( t_{1/2} = 0.56 \) d for non-poisoned water tank in late summer (Wakeham et al. 1983).
TABLE 2.1.1.31.1
Reported vapor pressures of *n*-pentadecane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\text{Stull 1947} & \quad \text{Camin & Rossini 1955} & \quad \text{Zwolinski & Wilhoit 1971} & \quad \text{Allemand et al. 1986} \\
\text{summary of literature data} & \quad \text{ebulliometry} & \quad \text{selected values} & \quad \text{gas saturation} \\
\text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} & \text{t/°C} & \text{P/Pa} \\
91.6 & 133.3 & 169.686 & 5532 & 135.8 & 1333 & 60.0 & 15.87 \\
121.0 & 666.6 & 180.919 & 8325 & 151.41 & 2666 & 72.84 & 35.60 \\
135.4 & 1333 & 188.905 & 10927 & 161.45 & 4000 & 81.53 & 64.13 \\
150.2 & 2666 & 206.866 & 19417 & 168.78 & 5333 & 94.31 & 148.0 \\
167.7 & 5333 & 219.982 & 26546 & 174.785 & 6666 & 111.0 & 394.0 \\
178.4 & 7999 & 235.150 & 43159 & 188.185 & 10666 & 136.0 & 1465 \\
194.0 & 13332 & 251.703 & 67061 & 194.949 & 13332 & & \\
216.1 & 26664 & 262.310 & 84081 & 207.872 & 19998 & & \\
242.8 & 53329 & 269.164 & 98106 & 217.641 & 26664 & & \\
270.5 & 101325 & 270.449 & 101069 & 225.582 & 33331 & & \\
\text{mp/°C} & 10 & \text{bp/°C} & 270.613 & & & & \\
\text{bp/°C} & 270.685 & & & & & & \\
\end{align*}
\]

- \( \log P = A - B/(T/K) \) (1)
- \( \log P = A - B/(C + t/°C) \) (2)
- \( \log P = A - B/(C + T/K) \) (3)
- \( \log P = A - B/(T/K) - C\log(T/K) \) (4)
- \( \ln \left( \frac{P}{P_{ref}} \right) = \left[ 1 - \frac{T}{T_{ref}} \right] \exp(a + bT + cT^2) \) (5) - Cox eq.

Stull 1947

- 91.6 133.3
- 121.0 666.6
- 135.4 1333
- 150.2 2666
- 167.7 5333
- 178.4 7999
- 194.0 13332
- 216.1 26664
- 242.8 53329
- 270.5 101325

Camin & Rossini 1955

- t/°C
- P/Pa
- 169.686 5532
- 180.919 8325
- 188.905 10927
- 206.866 19417
- 219.982 26546
- 235.150 43159
- 251.703 67061
- 262.310 84081
- 269.164 98106
- 270.449 101069

Zwolinski & Wilhoit 1971

- t/°C
- P/Pa
- 135.8 1333
- 151.41 2666
- 161.45 4000
- 168.78 5333
- 174.785 6666
- 179.859 7999
- 188.185 10666
- 194.949 13332
- 207.872 19998
- 217.641 26664
- 225.582 33331

Allemand et al. 1986

- t/°C
- P/Pa
- 60.0 15.87
- 72.84 35.60
- 81.53 64.13
- 94.31 148.0
- 111.0 394.0
- 136.0 1465

- mp/°C
- 10
- bp/°C
- 270.613

- bp/°C
- 270.685

- \( \Delta H_v/(kJ \text{ mol}^{-1}) \) at 25°C
- 76.15
- 10°C
- 49.45
FIGURE 2.1.1.31.1 Logarithm of vapor pressure versus reciprocal temperature for \( n \)-pentadecane.

\[ \log(P^2/\text{Pa}) \]

- Experimental data
- Stull 1947
- Zwolinski & Wilhoit 1971
- Ruzicka & Majer 1994

b.p. = 270.6 °C
m.p. = 9.95 °C
2.1.1.1.32  n-Hexadecane

Common Name: Hexadecane
Synonym: cetane
Chemical Name: \( n \)-hexadecane
CAS Registry No: 544-76-3
Molecular Formula: \( C_{16}H_{34}; \ CH_3(CH_2)_{14}CH_3 \)
Molecular Weight: 226.441
Melting Point (°C): 18.12 (Lide 2003)
Boiling Point (°C): 286.86 (Lide 2003)
Density (g/cm³):
0.77344, 0.76996 (20°C, 25°C, Camin et al. 1954; Dreisbach 1959)
0.7733 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
292.8 (20°C, calculated-density, Stephenson & Malanowski 1987)
362.2 (calculated-Le Bas molar volume at normal boiling point, Eastcott et al. 1988)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
81.35 (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
53.35, 51.46; 53.35 (18.15, 17.95°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
176.79, 165.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
6.28 \times 10^{-3} \text{ (shake flask, Franks 1966)}
2.1 \times 10^{-5} \text{ (extrapolated data of McAuliffe 1966, Coates et al. 1985)}
5.21 \times 10^{-5} \text{ (extrapolated from data of McAuliffe 1996, Eastcott et al. 1988)}
9.0 \times 10^{-4}, 4.0 \times 10^{-4} \text{ (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)}
2.33 \times 10^{-6} \text{ (calculated-TSA, Lande et al. 1985)}
0.0272 \text{ (calculated-molar volume correlation, Wang et al. 1992)}
4.95 \times 10^{-5} \text{ (calculated-molar volume and mp., Ruelle Kesselring 1997)}
Vapor Pressure (Pa at 25°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* \text{ (105.3°C, summary of literature data, temp range 105.3–287.5°C, Stull 1947)}
6945* \text{ (190.054°C, ebulliometry, measured range 190.054–286.704°C, Camin et al. 1954)}
13.33* \text{ (81.0°C, static method-Hg manometer, measured range 81.0–286.0°C, Myers & Fenske 1955)}
\log (P/mmHg) = 7.03044 – 1831.317/(154.528 + t/°C); temp range 190.0–286.8°C (Antoine eq., ebulliometry-manometer measurements, Camin et al. 1954)
0.14 \text{ (71.87°C, calculated-Antoine eq., Dreisbach 1959)}
0.221* \text{ (derived from compiled data, Zwolinski & Wilhoit 1971)}
\log (P/mmHg) = 7.02867 – 1830.51/(154.450 + t/°C); temp range 149.18–320.7°C (Antoine eq., Zwolinski & Wilhoit 1971)
\log (P/mmHg) = [-0.2185 \times 15405.5/(T/K)] + 8.956267; temp range 105.3–287.5°C (Antoine eq., Weast 1972–73)
0.092 \text{ (extrapolated-Antoine eq., Boublík et al. 1973, 1984)}
\log (P/mmHg) = 7.03519 – 1835.24/(t/°C + 154.968); temp range 188–285°C (Antoine eq. from exptl. data of Camin et al. 1945, Boublík et al. 1973)
\log (P/kPa) = 6.16189 – 1836.287/(t/°C + 155.125); temp range 190–287°C (Antoine eq. from exptl. data of Camin et al. 1954, Boublík et al. 1984)
log (P/mmHg) = 7.02867 – 1830.51/(154.45 + t/°C); temp range 149–321°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 6.77064 – 2273.168/(T/K – 80.252); temp range 323–425 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
log (P/kPa) = 6.15357 – 1830.57/(T/K – 118.7); temp range 467–563 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
log (P/mmHg) = 7.02967 – 1830.51/(t/°C + 154.45); temp range 149–321°C (Antoine eq., Dean 1992)
log (P/mmHg) = 99.1091 – 7.5333 × 10^3/(T/K) – 32.251·log (T/K) + 1.0453 × 10^{-2}·(T/K) + 1.2328 × 10^{-12}·(T/K)^2; temp range 291–721 K (vapor pressure eq., Yaws 1994)
0.191* (recommended, Ruzicka & Majer 1994)
In [(P/kPa)/(P_0/kPa)] = [1 – (T/K)/(T_0/K)]·exp{3.18271 – 2.002545 × 10^{-3}·(T/K) + 1.384476 × 10^{-6}·(T/K)^2}; reference state at P_0 = 101.325 kPa, T_0 = 559.978 K (Cox equation, Ruzicka & Majer 1994)
0.190 (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry’s Law Constant (Pa·m³/mol at 25°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 K_{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 K_{OA}:

Bioconcentration Factor, log BCF or log K_{b}:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volutilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, #data at other temperatures see reference:
  k_{OH} = 25.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 312 K (Atkinson 1989)
  k_{OH} = 25.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)
  k_{OH} = 23.0 × 10^{-12} cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation: microbial degradation t½ < 31 d by Pseudomonas sp. (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):

Half-Lives in the Environment:
TABLE 2.1.1.32.1
Reported vapor pressures of \( n \)-hexadecane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a)
\]

\[
\log P = A - \frac{B}{C + T/K} \quad (2) \\
\ln P = A - \frac{B}{C + T/K} \quad (2a)
\]

\[
\log P = A - \frac{B}{C + t/°C} \quad (3) \\
\ln P = A - \frac{B}{C + t/°C} \quad (3a)
\]

\[
\log P = A - \frac{B}{T/K} - C\cdot \log (T/K) \quad (4)
\]

\[
\ln (P/P_{\text{ref}}) = [1 - (T_{\text{ref}}/T)]\cdot \exp(a + bT + cT^2) \quad (5) - \text{Cox eq.}
\]

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<th>t/°C</th>
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\( \Delta H_v/(kJ \text{ mol}^{-1}) = \)

at 25°C \( 81.09 \)

at bp \( 51.21 \)

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data fitted to Wagner eq.

FIGURE 2.1.1.32.1 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: C\textsubscript{17}H\textsubscript{36}; CH\textsubscript{3}(CH\textsubscript{2})\textsubscript{15}CH\textsubscript{3}
Molecular Weight: 240.468
Melting Point (°C):
22 (Lide 2003)
Boiling Point (°C):
302 (Lide 2003)
Density (g/cm\textsuperscript{3}):
0.7780, 0.7745 (20°C, 25°C, Dreisbach 1959)
0.7780 (Weast 1982–83)
Molar Volume (cm\textsuperscript{3}/mol):
384.8 (calculated-Le Bas method at normal boiling point)
309.1 (20°C, calculated-density)
Enthalpy of Vaporization, \(\Delta H_V\) (kJ/mol):
61.65, 53.12 (25°C, bp, Dreisbach 1961)
86.47 (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
10.96, 40.17; 51.13 (1.15, 21.95°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
174.61, 175.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
5.5 \times 10^{-6} (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
0.0014 (reported as \(-\log S\) (mol/L) = 7.24, calculated-molar volume, Wang et al. 1992)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
log (P/mmHg) = 173.4039 –1.0943 × 10^4/(T/K) –59.212·log (T/K) + 2.0705 × 10^–2·(T/K) –1.3433 × 10^–12·(T/K)^2;

temp range 295–733 K (vapor pressure eq., Yaws 1994)
0.0627 (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry’s Law Constant (Pa m³/mol at 25°C): 5415 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{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 K_{oa}:

Bioconcentration Factor, log BCF or log K_{bi}:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constant, k, and Half-Lives, t:\nVolatilization: volatilization k = 1.23 d⁻¹ with a water column t_{50} = 0.6 d at 6–18°C in spring; k = 0.79 d⁻¹ with a water column t_{50} = 0.9 d at 20–22°C in summer; k = 0.14 d⁻¹ with a water column t_{50} = 5.0 d at 3–7°C in winter for mesocosm experiments in coastal marine environment; volatilization k = 0.359 d⁻¹ with a water column t_{50} = 1.9 d with HgCl poisoned water tank and k = 1.362 d⁻¹ with a water column t_{50} = 0.51 d for non-poisoned water tank in late summer (Wakeham et al. 1983).

Photolysis:
Oxidation:
Hydrolysis:
Biodegradation: microbial degradation t_{50} < 31 d by Pseudomonas sp. (Setti et al. 1993)
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):

Half-Lives in the Environment:
Surface water: water column t_{50} = 0.6 d at 6–18°C, in spring; t_{50} = 0.9 d at 20–22°C, in summer; t_{50} = 5.0 d at 3–7°C, in winter for mesocosm experiment in coastal marine environment; t_{50} = 1.9 d with HgCl poisoned water tank and t_{50} = 0.51 d for non-poisoned water tank in late summer (Wakeham et al. 1983).

### TABLE 2.1.1.33.1
Reported vapor pressures of n-heptadecane at various temperatures and the coefficients for the vapor pressure equations

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### TABLE 2.1.1.1.33.1 (Continued)

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**FIGURE 2.1.1.1.33.1** Logarithm of vapor pressure versus reciprocal temperature for \( n \)-heptadecane.
Common Name: Octadecane
Synonym:
Chemical Name: \( n \)-octadecane
CAS Registry No: 543-45-3
Molecular Formula: \( C_{18}H_{38} \); \( \text{CH}_3(\text{CH}_2)_{16}\text{CH}_3 \)
Molecular Weight: 254.495
Melting Point (°C):
28.2 (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
316.3 (Lide 2003)
Density (g/cm³):
0.7819, 0.7785 (20°C, 25°C, Dreisbach 1959)
0.7768 (Weast 1982–83)
Molar Volume (cm³/mol):
325.5 (20°C, calculated-density)
407.0 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
Enthalpy of vaporization, \( \Delta H_v \) (kJ/mol):
90.824, 54.84 (25°C, bp, Dreisbach 1959)
91.6 (25°C, Piacente et al. 1994)
91.44 (298.15K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
61.384 (Dreisbach 1959)
61.13 (28°C, Piacente et al. 1994)
61.5 (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
204.6, 184.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \text{ J/mol K} \), F: 0.930 (mp at 28.2°C)
Water Solubility (g/m³ or mg/L at 25°C):
7.75 × 10⁻³ (Baker 1959)
2.1 × 10⁻³; 8.0 × 10⁻⁴ (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
1.40 × 10⁻⁶ (extrapolated from data of McAuliffe 1966, Coates et al. 1988)
4.05 × 10⁻⁶ (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)
Vapor Pressure (Pa at 25°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* (119.6°C, summary of literature data, temp range 119.6–317.0°C, Stull 1947)
26.66* (102.4°C, static method-Hg manometer, measured range 102.4–313°C, Myers & Fenske 1955)
\[ \log (P/\text{mmHg}) = 7.0156 - 1883.73/(139.46 + t/°C); \text{temp range 201–387}°\text{C} \] (Antoine eq. for liquid state, Dreisbach 1959)
1333* (172.3°C, derived from compiled data, temp range 172.3–316.3°C, Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 7.0022 - 1894.3/(143.3 + t/°C); \text{temp range 172.3–352}°\text{C} \] (Antoine eq., Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = \text{–0.2185} \times 15447.0/(T/K) + 8.619864; \text{temp range 119.6–317}°\text{C} \] (Antoine eq., Weast 1972–73)
0.013 (extrapolated-Antoine eq., Boublik et al. 1973)
\[ \log (P/\text{mmHg}) = 7.14067 - 2012.745/(t/°C + 155.492); \text{temp range 174–317}°\text{C} \] (Antoine eq., Boublik et al. 1973)
0.0259 (liquid \( P_L \), extrapolated-Antoine eq., Macknick & Prausnitz 1979)
0.220* (45.0°C, gas saturation, measured range 45.0–88.10°C, Macknick & Prausnitz 1979)
\[ \ln (P_L/\text{mmHg}) = 25.548 - 10165/(T/K); \text{temp range 45–88.1}°\text{C} \] (Antoine eq. on exptl. data, gas saturation, liquid state, Macknick & Prausnitz 1979)
Aliphatic and Cyclic Hydrocarbons

log (P/kPa) = 6.27065 – 2016.983/(t/°C + 155.924); temp range 174–317°C (Antoine eq., Boublik et al. 1984)

log (P/mmHg) = 7.0022 – 1894.3/(t/°C + 143.30); temp range 172–352°C (Antoine eq., Dean 1992)

1.15* (62.04°C, gas saturation, measured temp range 335.19–439.82 K, Allemand et al. 1986)

0.0261 (extrapolated-Antoine eq.-I, liquid, Stephenson & Malanowski 1987)

log (P/kPa) = 10.18833 – 4404.095/(T/K); temp range 310–361 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

log (P/kPa) = 6.1392 – 1894.3/(T/K – 129.85); temp range 501–550 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.0022 – 1894.3/(t/°C + 143.30); temp range 172–352°C (Antoine eq., Dean 1992)

256.6* (139.919°C, static-differential pressure, measured range 139.919–314.982°C, Morgan & Kobayashi 1994)

0.02007* (recommended, temp range 396–500 K, Ruzicka & Majer 1994)

Henry’s Law Constant (Pa·m3/mol at 25°C or as indicated):

1013 (15°C, 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 K_{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 K_{oa}:

Bioconcentration Factor, log BCF or log K_{bi}:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Photolysis:

Hydrolysis:

Biodegradation: degradation rate constant of about 0.66 d^{-1} in a microcosm experiment. (Wakeham et al. 1986); microbial degradation t_{1/2} < 31 d by Pseudomonas sp. (Setti et al. 1993).

Biotransformation:

Biocumulation and Uptake and Elimination Rate Constants (k_{i} and k_{j}):

Half-Lives in the Environment:

Surface water: an estimated t_{1/2} = 1.5 d in Rhine River for a first order reduction process in river water (Zoeteman et al. 1980)

t_{1/2} ~ 23 d in a seawater microcosm experiment (Wakeham et al. 1986).
TABLE 2.1.1.34.1
Reported vapor pressures of n-octadecane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\log P = A - \frac{B}{(C + t/°C)} \quad (2) \\
\log P = A - \frac{B}{(C + T/K)} \quad (3) \\
\log P = A - \frac{B}{(T/K)} - C \log (T/K) \quad (4) \\
\ln \left(\frac{P}{P_{ref}}\right) = \left[1 - \frac{T_{ref}}{T}\right] \exp(a + bT + cT^2) \quad (5) \text{- Cox eq.}
\]

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\[\Delta H_v/(kJ \text{ mol}^{-1}) =\]
\[\text{at 25°C} \quad 90.8\]
\[\text{at bp} \quad 54.48\]
TABLE 2.1.1.34.1 (Continued)

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- $10^b/K^{-1}$
- $10^c/K^{-2}$

- data fitted to Wagner eq.

FIGURE 2.1.1.34.1 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: \( C_{20}H_{42}; CH_3(CH_2)_{18}CH_3 \)
Molecular Weight: 282.547
Melting Point (°C):
36.6  (Lide 2003)
Boiling Point (°C):
334.8  (Chirico et al. 1989)
Density (g/cm³):
0.7887, 0.7853  (20°C, 25°C, Dreisbach 1959)
0.7886  (Weast 1982–83)
Molar Volume (cm³/mol):
451.4  (calculated-Le Bas molar volume at normal boiling point)
358.2  (20°C, calculated-density)
358  (Wang et al. 1992)
Enthalpy of vaporization, \( \Delta H_v \) (kJ/mol):
63.93; 64.35  (exptl., calculated, Macknick & Prausnitz 1979b)
100.9; 110  (25, 94°C, Piacente et al. 1994)
101.81  (298.15 K, recommended, Ruzicka & Majer 1994)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
69.875  (Dreisbach 1959)
69.5  (Piacente et al. 1994)
67.8  (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
219.6, 203.1  (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), \( F \): 0.769 (mp at 36.6°C)
Water Solubility (g/m³ or mg/L at 25°C):
1.9 × 10⁻³, 8.0 × 10⁻⁴  (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
1.10 × 10⁻³  (extrapolated from data of McAuliffe 1966, Coates et al. 1985)
3.11 × 10⁻³  (extrapolated from data of McAuliffe 1966, Eastcott et al. 1985)
Vapor Pressure (Pa at 25°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*  (121.9°C, static method-Hg manometer, measured range 121.9–343.0°C, Myers & Fenske 1955)
\log (P/mmHg) = 7.0225 – 1948.7/(127.8 + t/°C), temp range: 224–417°C, (Antoine eq. for liquid state, Dreisbach 1959)
1333*  (198.3°C, derived from compiled data, temp range 198.3–343.8°C, Zwolinski & Wilhoit 1971)
\log (P/mmHg) = 7.1522 – 2032.7/(132.1 + t/°C); temp range:198.3–379°C (Antoine eq., Zwolinski & Wilhoit 1971)
0.41*  (71.5°C, \( P_L \), gas saturation-IR, Macknick & Prausnitz 1979)
\ln (P_L/mmHg) = 26.849 – 11230/(T/K); temp range: 71.15–107.3°C, (Antoine eq., gas saturation, liquid state, Macknick & Prausnitz 1979)
\log (P_L/kPa) = 10.7737 – 4872.63/(T/K); temp range: 344–380 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
\log (P_L/kPa) = 6.2771 – 2032.7/(T/K – 141.05); temp range 528–620 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
0.201*  (79.97°C, pressure gauge, measured range 90.07–194.21°C, Sasse et al. 1988)
\[
\log (P/\text{mmHg}) = 7.95834 - 2665.762/(t/°C + 167.047); \quad \text{(Antoine eq. derived from exptl. data, liquid phase, pressure gauge measurement, Sasse et al. 1988)}
\]

15.6* (115°C, inclined piston measurement, temp range 115–215°C, Chirico et al. 1989)

\[
\ln (P/\text{kPa}) = 19.36 - 9083/(T/K); \quad \text{temp range 406–472 K (transpiration method, Piacente et al. 1991)}
\]

\[
\ln (P/\text{kPa}) = 22.53 - 10649/(T/K); \quad \text{temp range 345–393 K (torsion method, Piacente et al. 1991)}
\]

\[
\ln (P/\text{kPa}) = 18.10 - 7889/[(T/K) + 32]; \quad \text{temp range 315–472 K (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)}
\]

\[
\log (P/\text{mmHg}) = 7.1522 - 2032.1/(t/°C + 132.10); \quad \text{temp range 198–379°C (Antoine eq., Dean 1992)}
\]

0.32*, 0.641 (74, 78°C, torsion-effusion method, measured temp range 74–115°C, Piacente et al. 1994)

\[
\log (P/\text{kPa}) = 13.37 - 5785/(T/K); \quad \text{temp range 351–384 K (torsion-effusion, Antoine eq., Piacente et al. 1994)}
\]

\[
\log (P/\text{kPa}) = 12.96 - 5709/(T/K); \quad \text{temp range 347–389 K (torsion-effusion, Antoine eq., Piacente et al. 1994)}
\]

\[
\log (P/\text{kPa}) = 13.16 - 5747/(T/K); \quad \text{temp range ~ 347–388 K, } \Delta H_v = 110 \text{ kJ mol}^{-1} \text{ (selected Antoine eq. based on exptl. data, torsion-effusion method, Piacente et al. 1994)}
\]

0.002091* (recommended, Ruzicka & Majer 1994)

\[
\ln \left[\frac{(P/\text{kPa})/(P_o/\text{kPa})}{(P'/\text{kPa})/(P_o/\text{kPa})}\right] = \left[1 - \left(\frac{T_o}{K}\right)/(T/K)\right] \cdot \exp\left\{3.31181 - 2.102218 \times 10^{-3} \cdot (T/K) + 1.348780 \times 10^{-6} \cdot (T/K)^2\right\};
\]

\[\text{reference state at } P_o = 101.325 \text{ kPa, } T_o = 617.415 \text{ K (Cox equation, Ruzicka & Majer 1994)}\]

\[
\log (P/\text{mmHg}) = 19.4193 - 5.8699 \times 10^3/(T/K) - 44.282 \cdot \log (T/K) - 1.2606 \times 10^{-2} \cdot (T/K) + 5.2241 \times 10^{-6} \cdot (T/K)^2;
\]

\[\text{temp range 310–767 K (vapor pressure eq., Yaws 1994)}\]

0.00209* (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry’s Law Constant (Pa·m³/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 \(K_{OW}\):

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 \(K_{OA}\):

Bioconcentration Factor, log BCF or log \(K_B\):

Sorption Partition Coefficient, log \(K_{OC}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):

Biodegradation: microbial degradation \(t_{1/2} < 31\) d by \textit{Pseudomonas} sp. (Setti et al. 1993)

Half-Lives in the Environment:
### TABLE 2.1.1.35.1
Reported vapor pressures of eicosane at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\ln P = A - \frac{B}{C/T/K} \quad (3a) \\
\log P = A - \frac{B}{T/K} - C \log (T/K) \quad (4) \\
\ln (P/P_{ref}) = [1 - (T_{ref}/T)] \exp(a + bT + cT)^2 \quad (5)
\]

1. Myers & Fenske 1955

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\[ \Delta H_v/(kJ \text{ mol}^{-1}) = \]

at 25°C 100.8
at bp 57.49
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3. Piacente et al. 1991 (cont'd)

Knudsen method

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**eq. for run a**

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By weighing the slopes and intercepts of above 2 eq., selected vapor pressure eq. eq. 1 P/kPa mid-cut

298.15 K

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data fitted to Wagner eq.
FIGURE 2.1.1.35.1 Logarithm of vapor pressure versus reciprocal temperature for \( n \)-eicosane.
2.1.1.1.36  n-Tetracosane

Common Name: Tetracosane
Chemical Name: n-tetracosane
CAS Registry No: 646-31-1
Molecular Formula: C_{24}H_{50}; CH_3(CH_2)_{22}CH_3
Molecular Weight: 338.654
Melting Point (°C): 50.4 (Lide 2003)
Boiling Point (°C): 391.3 (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³):
- 0.7991, 0.7958 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
- 540.2 (calculated-Le Bas method at normal boiling point)
- 423.8 (20°C, calculated-density)
Enthalpy of vaporization, ∆HV (kJ/mol):
- 126 (132°C, Piacente et al. 1994)
- 121.9 (calculated, Chickos & Hanshaw 2004)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
- 54.9 (Dreisbach 1959; Piacente et al. 1994)
- 31.3, 54.89; 86.19 (48.15, 50.95°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
- 266.79, 240.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
- Fugacity Ratio at 25°C (assuming ∆Sfus = 56 J/mol K), F: 0.563 (mp at 50.4°C)

Water Solubility (g/m³ or mg/L at 25°C):
- 5.8 × 10⁻¹⁰ (extrapolated from data of McAuliffe 1966, Coates et al. 1985)

Vapor Pressure (Pa at 25°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* (183.8°C, summary of literature data, temp range 183.8–386.4°C, Stull 1947)
- log (P/mmHg) = 7.53923 – 2591.9/(165.1 + t°C); temp range 260–500°C (Antoine eq. for liquid state, Dreisbach 1959)
- log (P/mmHg) = 7.0976 – 2112.0/(109.6 + t°C) (Antoine eq., Kudchadker & Zwolinski 1966)
- 66.66* (175.9°C, derived from compiled data, temp range 175.9–391.3°C, Zwolinski & Wilhoit 1971)
- log (P/mmHg) = 7.0976 – 2112.0/(109.6 + t°C); temp range 175.9–391.3°C (Antoine eq., Zwolinski & Wilhoit 1971)
- log (P/mmHg) = –0.2185 × 19642.5/(T/K) + 9.408166; temp range 183.8–386.4°C (Antoine eq., Weast 1972–73)
- log (P/kPa) = 6.44051 – 2289.02/(T/K – 147.92); temp range 498–573 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
- 0.253* (100.26°C, pressure gauge, Sasse et al. 1988)
- log (P/mmHg) = 7.17666 – 2243.665/(t°C + 126.236); temp range 100.26–149.23°C (Antoine eq. derived from exptl. data, liquid phase, Sasse et al. 1988)
- log (P/kPa) = (8.76 ± 0.50) – (4501 ± 250)/(T/K); temp range 451–497 K (Antoine eq. from exptl. data, transpiration method, Piacente & Scardala 1990; quoted, Pompilii & Piacente 1990)
- ln (P/kPa) = 21.25 – 10946/(T/K); temp range 501–523 K (transpiration method, Piacente et al. 1991)
- ln (P/kPa) = 25.35 – 12399/(T/K); temp range 376–438 K (torsion method, Piacente et al. 1991)
- ln (P/kPa) = 18.38 – 8349/[T(K) + 58]; temp range 343–523 K (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)

0.721°, 0.801 (114, 115°C, torsion-effusion, measured range 386–425 K, Piacente et al. 1994)

log (P/kPa) = 13.57 – 6459/(T/K); temp range 388–413 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 14.25 – 6726/(T/K); temp range 387–423 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.92 – 6591/(T/K); temp range 386–425 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.96 – 6608/(T/K); temp range ~ 386–425 K, \( \Delta H_v = 126 \text{ kJ mol}^{-1} \) (selected Antoine eq. based on expl. data, torsion-effusion method, Piacente et al. 1994)

3.30 × 10⁻⁵ (quoted from Daubert & Danner 1997, Goss & Schwarzenbach 1999)

2.37 × 10⁻⁵ (GC-retention time correlation, Chickos & Hanshaw 2004)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, \( \log K_{ow} \):

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, \( \log K_{oa} \):

Bioconcentration Factor, \( \log BCF \) or \( \log K_{bi} \):

Sorption Partition Coefficient, \( \log K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Biodegradation: microbial degradation \( t_{1/2} < 31 \text{ d} \) by *Pseudomonas* sp. (Setti et al. 1993)

Half-Lives in the Environment:

**TABLE 2.1.1.36.1**

Reported vapor pressures of tetracosane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\ln P &= A - B/(C + t/K) \quad (3a) \\
\log P &= A - B/(T/K) - C \log (T/K) \quad (4)
\end{align*}
\]

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<th>( t/°C )</th>
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for transpiration data:

| **t/°C** | **P/Pa** | **t/°C** | **P/Pa** | **t/°C** | **P/Pa** |
| runs C  | 123.85 2.951 | 126.85 3.981 | 130.85 3.548 |
|         | 126.85 3.981 | 134.8513885 4.577 |
|         | 133.85 5.888 | 139.85 5.888 |
|         | 135.85 7.079 | 140.85 6.457 |
|         | 137.85 8.128 | 142.85 9.333 |
|         | 139.85 8.128 | 144.85 10.47 |
|         | 142.85 9.333 | 147.85 12.88 |
### Table 2.1.36.1 (Continued)

#### Piacente et al. 1990 (cont'd)

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<td>$\Delta H_v/(kJ\ mol^{-1}) = 86 ± 5$</td>
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#### Piacente et al. 1991

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#### Piacente et al. 1991 (cont'd)

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#### Piacente et al. 1994

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#### Morgan & Kobayashi 1994

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### TABLE 2.1.1.36.1 (Continued)

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<td>314.820</td>
<td>17460</td>
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Data fitted to Wagner eq.

### FIGURE 2.1.1.36.1

Logarithm of vapor pressure versus reciprocal temperature for $n$-tetracosane.

- Experimental data
- Stull 1947
- Zwolinski & Wilhoit 1971

- B.p. = 391.3 °C
- M.p. = 50.4 °C

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2.1.1.1.37 n-Hexacosane

Common Name: Hexacosane
Synonym: cerane
Chemical Name: \( n \)-hexacosane
CAS Registry No: 631-01-3
Molecular Formula: \( C_{26}H_{54} \); \( CH_3(CH_2)_{24}CH_3 \)
Molecular Weight: 366.707
Melting Point (°C):
56.1 (Lide 2003)
Boiling Point (°C):
412.2 (Dreisbach 1959; Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³):
0.8032, 0.7998 (20°C, 25°C, Dreisbach 1959)
0.8032 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
584.6 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)
456.6 (20°C, calculated-density)
457 (Wang et al. 1992)
Enthalpy of vaporization, \( \Delta H_v \) (kJ/mol):
64.806 (bp, Dreisbach 1959)
131.2 (calculated, Chickos & Hanshaw 2004)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
32.3, 59.5; 95.3 (53.35, 56.35°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
289.03, 259.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \text{ J/mol K} \)): F: 0.495 (mp at 56.1°C)
Water Solubility (g/m³ or mg/L at 25°C):
1.7 × 10⁻³; 1.0 × 10⁻⁴ (shake flask-GC, distilled water; seawater, Sutton & Calder 1974)
1.33 × 10⁻¹⁰ (extrapolated from data of McAuliffe 1966, Eastcott et al. 1988)
Vapor Pressure (Pa at 25°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* (204.0°C, summary of literature data, temp range 204.0–399.8°C, Stull 1947)
\( \log (P/\text{mmHg}) = 7.57689 − 2692.73/(161.2 + t/°\text{C}) \); temp range 278–500°C (Antoine eq. for liquid state, Dreisbach 1959)
\( \log (P/\text{mmHg}) = 7.1096 − 2164.3/(99.6 + t/°\text{C}) \) (Antoine eq., Kudchadker & Zwolinski 1966)
66.66* (192.5°C, derived from compiled data, temp range 192.5–412.2°C, Zwolinski & Wilhoit 1971)
\( \log (P/\text{mmHg}) = 7.1096 − 2164.3/(99.6 + t/°\text{C}) \); temp range 192.6–412.2°C (Antoine eq., Zwolinski & Wilhoit 1971)
\( \log (P/\text{mmHg}) = −0.2185 \times 21605.7/(T/K) + 9.899820; \) temp range 204–399.8°C (Antoine eq., Weast 1972–73)
\( \log (P_\text{L}/\text{kPa}) = 6.2345 − 2164.3/(T/K – 173.55); \) temp range 466–685 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
\( \log (P_\text{L}/\text{kPa}) = 9.44384 − 4935.969/(T/K); \) temp range 478–530 K (Antoine eq., liquid, Stephenson & Malanowski 1987)
\( \log (P_\text{L}/\text{kPa}) = (9.93 \pm 0.50) − (5168 \pm 200)/(T/K); \) temp range 455–519 K, (Antoine eq. from exptl. data, transpiration, Piacente & Scardala 1990; Pompili & Piacente 1990)
\( \ln (P/\text{kPa}) = 18.63 − 9892/(T/K); \) temp range 506–546 K (transpiration method, Piacente et al. 1991)
\( \ln (P/\text{kPa}) = 28.91 − 14285/(T/K); \) temp range 391–442 K (torsion method, Piacente et al. 1991)
\( \ln (P/\text{kPa}) = 17.76 − 8050/(T/K) + 72; \) temp range 356–546 K (transpiration, torsion and Knudsen methods, Antoine eq., Piacente et al. 1991)
\( \log (P/\text{kPa}) = 14.50 − 7084/(T/K); \) temp range 420–437 K (torsion-effusion, Antoine eq., Piacente et al. 1994)
log (P/kPa) = 13.75 – 6765/(T/K); temp range 391–433 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 13.65 – 6748/(T/K); temp range 392–431 K (torsion-effusion, Antoine eq., Piacente et al. 1994)

log (P/kPa) = 14.01 – 6682/(T/K); temp range ~ 392–437 K, \( \Delta H_v = 132 \text{ kJ mol}^{-1} \) (selected Antoine eq. based on exp. data, torsion-effusion method, Piacente et al. 1994)

5.03 \times 10^{-6} \text{ (quoted from Daubert & Danner 1997, Goss & Schwarzenbach 1999)}

2.82 \times 10^{-6} \text{ (GC-retention time correlation, Chickos & Hanshaw 2004)}

Henry’s Law Constant (Pa·m³/mol):

21200 \text{ (calculated-P/C, Eastcott et al. 1988)}

Octanol/Water Partition Coefficient, log \( K_{ow} \):

13.0, 11.4 \text{ (calculated-fragment const., calculated-molar volume correlation, Wang et al. 1992)}

Octanol/Air Partition Coefficient, log \( K_{oa} \):

Bioconcentration Factor, log BCF or log \( K_b \):

Sorption Partition Coefficient, log \( K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Biodegradation: microbial degradation \( t_{1/2} < 31 \text{ d} \) by \textit{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**

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<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( t/°C )</th>
<th>( P/Pa )</th>
<th>( t/°C )</th>
<th>( P/Pa )</th>
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<tbody>
<tr>
<td>204.0</td>
<td>133.3</td>
<td>192.5</td>
<td>66.66</td>
<td>run A</td>
<td>187.85</td>
<td>64.57</td>
<td>run C</td>
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<tr>
<td>240.0</td>
<td>666.6</td>
<td>204.8</td>
<td>133.3</td>
<td>194.35</td>
<td>74.13</td>
<td>188.85</td>
<td>54.95</td>
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<td>257.4</td>
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<td>266.6</td>
<td>197.35</td>
<td>91.20</td>
<td>193.35</td>
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<td>275.8</td>
<td>2666</td>
<td>138.0</td>
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<td>295.2</td>
<td>5333</td>
<td>254.6</td>
<td>527.75</td>
<td>198.35</td>
<td>97.72</td>
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<td>307.8</td>
<td>7999</td>
<td>412.2</td>
<td>101325</td>
<td>199.85</td>
<td>109.65</td>
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<td>53329</td>
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<td>162.2</td>
<td>206.85</td>
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<td>P/mmHg</td>
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<tr>
<td>374.5</td>
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<td>bp/°C</td>
<td>412.2</td>
<td>208.85</td>
<td>162.2</td>
<td>206.85</td>
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<td>eq. 2</td>
<td>P/mmHg</td>
<td>211.85</td>
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<td>210.85</td>
<td>229.1</td>
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(Continued)
TABLE 2.1.1.37.1 (Continued)

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<td>t/°C</td>
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<td>t/°C</td>
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<td>B</td>
<td>5355 ± 198</td>
<td>243.35</td>
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<td>for temp range: 461–488 K</td>
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<tr>
<td></td>
<td>242.35</td>
<td>5168 ± 200</td>
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| ∆HV/(kJ mol–1) = | |
| for temp range: 475.5–508 K | at 488 K | 99 ± 4 |

2.

<table>
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<td>t/°C P/Pa</td>
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<td>B 9892 ± 552</td>
<td>136.35</td>
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<td>A 14285 ± 345</td>
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3.

Piacente et al. 1991 (cont’d)

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<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
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<td>83 0.01995</td>
<td>146.85</td>
<td>4.01</td>
<td>117.85</td>
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<td>eq. 3a P/kPa</td>
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<td>A 17.76 ± 0.46</td>
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<td>13.3</td>
<td>157.85</td>
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<td>B 8050 ± 460</td>
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<td>C 72 ± 10</td>
<td>163.85</td>
<td>18.9</td>
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<td>eq. 1 P/kPa</td>
<td>eq. 1 P/kPa</td>
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<tr>
<td>A</td>
<td>13.75 ± 0.29</td>
<td>A</td>
<td>13.65 ± 0.29</td>
</tr>
<tr>
<td>B</td>
<td>14.50 ± 0.36</td>
<td>B</td>
<td>6765 ± 119</td>
</tr>
<tr>
<td>C</td>
<td>7084 ± 153</td>
<td>B</td>
<td>6748 ± 120</td>
</tr>
<tr>
<td>temp range: 391–433 K</td>
<td>temp range: 392–431 K</td>
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</tr>
<tr>
<td><strong>∆Hfus/(kJ mol⁻¹)</strong> = 60.70</td>
<td>overall vapor pressure eq.</td>
<td><strong>∆Hfus/(kJ mol⁻¹)</strong> = 59.9</td>
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</tr>
<tr>
<td><strong>∆Hsub/(kJ mol⁻¹)</strong> = 177.2</td>
<td>at 298.15 K</td>
<td>at 298.15 K</td>
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</tr>
<tr>
<td>at 298.15 K</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>temp range: 420–437 K</td>
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</tbody>
</table>
FIGURE 2.1.1.37.1 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: C₅H₁₀
Molecular Weight: 70.133
Melting Point (°C):
-93.4 (Lide 2003)
Boiling Point (°C):
49.3 (Lide 2003)
Density (g/cm³ at 20°C):
0.7457 (Weast 1984)
0.7454, 0.7440 (20°C, 25°C, Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
94.10 (20°C, calculated-density; McAuliffe 1966)
99.5 (calculated-Le Bas method at normal boiling point, Abernethy et al. 1988; Mackay & Shiu 1990)
Enthalpy of Vaporization, ∆HV (kJ/mol):
28.527, 27.296 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
0.609 (Riddick et al. 1986)
4.9, 0.34, 0.60; 5.84 (–151.15, –135.15, –93.45°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
45.96, 40.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Pierotti & Liabastre 1972)
164 (shake flask-GC, Krzyzanowska & Szeliga 1978)
156* (shake flask-GC, Groves 1988)
166* (IUPAC “tentative” best, IUPAC Solubility Data Series, Shaw 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
27250* (14.25°C, static method-manometry, measured range –47.24 to 14.25°C, Ashton et al. 1943)
34890* (20.2°C, ebulliometry-manometer, measured range 15.7–50°C, Willingham et al. 1945)
log (P/mmHg) = 6.87798 – 1119.208/(230.738 + t°C); temp range 15.7–50.0°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
43150* (Antoine eq. regression, temp range –68 to 49.4°C, Stull 1947)
42330 (calculated from exptl. determined data, Dreisbach 1955; quoted, Hine & Mookerjee 1975)
log (P/mmHg) = 6.88676 – 1124.162/(231.361 + t°C); temp range –25 to 110°C (Antoine eq. for liquid state, Dreisbach 1955)
29036* (selected exptl. data, temp range –39 to 230°C, Pasek & Thodos 1962)
log (P/mmHg) = 6.88676 – 1124.162/(231.361 + t/°C); temp range –40.4 to 71.6°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = \left[-0.2185 \times 7411.1/(T/K)\right] + 7.940722; temp range –68 to 49.3°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = \left[1– 322.386/(T/K)\right] \times 10^{0.818603 – 7.52365 \times 10–4\cdot(T/K) + 8.27395 \times 10–7\cdot(T/K)^2}; temp range: 190.20–503.20 K (Cox eq., Chao et al. 1983)

log (P/kPa) = 6.04584 – 1142.30/(233.463 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 6.08918 – 1174.132/(–34.864 + T/K); temp range 322–384 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.41769 – 1415.096/(–0.66 + T/K); temp range 381–455 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 6.77782 – 1749.65/(48.533 + T/K); temp range 179–512 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

log KAW = 5.162 – 1302/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log KOW:

2.05 (calculated-π 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 KOA:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{O}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression:

$k_{\text{O}(3\text{P})} = 1.30 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with O(3P) (Herron & Huie 1973)

$k_{\text{OH}} = (4.72 \pm 0.28) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}} (\text{calc}) = 5.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (relative rate method, Darnall et al. 1978)

$k_{\text{OH}} = 5.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979)

$k_{\text{OH}} = 5.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{\text{O}(3\text{P})} = 1.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with O(3P) atoms at room temp. (Gaffney & Levine 1979)

$k_{\text{OH}} = 6.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and $5.18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and $5.24 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson 1985)

$k_{\text{OH}} = (3.12 \pm 0.23) \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (flash photolysis-resonance absorption technique, Jolly et al. 1985)

$k_{\text{OH}} = 5.02 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–491 K (Droege & Tully 1987)

$k_{\text{OH}}^\# = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K with an estimated lifetime of 27 h in summer daylight (Altshuller 1991)

$k_{\text{OH}}^\# = 5.02 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{\text{OH}}^\# = 4.83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} \sim 2.4–24$ h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

photooxidation reaction rate constant $k = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Solubility</th>
<th>Temperature</th>
<th>Solubility</th>
<th>Temperature</th>
<th>Solubility</th>
<th>Temperature</th>
<th>Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>shake flask-GC/FID</strong></td>
<td><strong>shake flask-GC/FID</strong></td>
<td><strong>IUPAC “tentative” values</strong></td>
<td><strong>calc-recommended LLE data</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m³</td>
<td>t/°C</td>
<td>S/g·m³</td>
<td>t/°C</td>
<td>S/g·m³</td>
<td>t/°C</td>
<td>S/g·m³</td>
</tr>
<tr>
<td>5.11</td>
<td>338.6</td>
<td>25.0</td>
<td>160</td>
<td>5</td>
<td>339</td>
<td>25</td>
<td>168</td>
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<td>15.21</td>
<td>341.7</td>
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<td>163</td>
<td>15</td>
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<td>40.1</td>
<td>175</td>
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<tr>
<td>25.11</td>
<td>341.9</td>
<td>55.7</td>
<td>180</td>
<td>25</td>
<td>156</td>
<td>55.7</td>
<td>195</td>
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<tr>
<td>35.21</td>
<td>368.5</td>
<td>99.1</td>
<td>296</td>
<td>30</td>
<td>160</td>
<td>99.1</td>
<td>343</td>
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<tr>
<td>45.21</td>
<td>341.5</td>
<td>118.0</td>
<td>372</td>
<td>40</td>
<td>350</td>
<td>118</td>
<td>468</td>
</tr>
<tr>
<td>∆H$_{\text{sol}}$(kJ mol$^{-1}$) = –2.50</td>
<td>137.3</td>
<td>611</td>
<td>60</td>
<td>500</td>
<td>137.3</td>
<td>701</td>
<td></td>
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<tr>
<td>25°C</td>
<td>153.1</td>
<td>792</td>
<td>80</td>
<td>750</td>
<td>153.1</td>
<td>974</td>
<td></td>
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<tr>
<td>∆H$_{\text{sol}}$(kJ mol$^{-1}$) = –2.80</td>
<td>100</td>
<td>1100</td>
<td>100</td>
<td>1100</td>
<td>100</td>
<td>1100</td>
<td></td>
</tr>
<tr>
<td>25°C</td>
<td>120</td>
<td>1600</td>
<td>120</td>
<td>1600</td>
<td>120</td>
<td>1600</td>
<td></td>
</tr>
<tr>
<td>140</td>
<td>2600</td>
<td>140</td>
<td>2600</td>
<td>140</td>
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<td>160</td>
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<td>6700</td>
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<td>6700</td>
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<td>200</td>
<td>14000</td>
<td>200</td>
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</tr>
</tbody>
</table>

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**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

\[
\begin{align*}
\text{log } P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\text{log } P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\text{log } P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (3) \\
\text{log } P &= A - \frac{B}{T/K} - C \cdot \log (T/K) + D \cdot [P/(T/K)]^2 \quad (4) \\
\text{log } P &= A - \frac{B}{T(K)} - C \cdot \log (T/K) + D \cdot 10^{-3}(T/K) - E \cdot 10^{-8}(T/K)^2 \quad (5) \\
\text{log } P &= A + \frac{B}{T(K)} + C \cdot \log (T/K) + D \cdot P/(T/K)^2 \quad (6)
\end{align*}
\]

1. Ashton et al. 1943  
Willingham et al. 1945  
Stull 1947  
Pasek & Thodos 1962

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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</thead>
<tbody>
<tr>
<td>–47.24</td>
<td>830.6</td>
<td>–15.707</td>
<td>28956</td>
<td>–68.0</td>
<td>133.3</td>
<td>–93.62</td>
<td>49.20</td>
</tr>
<tr>
<td>–38.35</td>
<td>1570</td>
<td>20.196</td>
<td>34892</td>
<td>–49.6</td>
<td>666.6</td>
<td>9.335</td>
<td>21949</td>
</tr>
<tr>
<td>–31.63</td>
<td>2446</td>
<td>25.598</td>
<td>43322</td>
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<td>15.722</td>
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<tr>
<td>–24.7</td>
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<td>–30.1</td>
<td>2666</td>
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<td>97608</td>
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<tr>
<td>–18.6</td>
<td>5360</td>
<td>37.119</td>
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<td>–12.91</td>
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<td>9.33</td>
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<td>49.587</td>
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<td>101325</td>
<td>49.307</td>
<td>9.33</td>
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<tr>
<td>14.25</td>
<td>27250</td>
<td>50.031</td>
<td>103921</td>
<td>mp/°C</td>
<td>–93.7</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

bp/°C | 49.20 | mp/°C | –93.62 |

\begin{align*}
eq 6 & \quad \text{P/mmHg} \quad \text{eq. 2} \quad \text{P/mmHg} \\
A & \quad 30.957385 \quad A \quad 6.87798 \\
B & \quad 2298.386 \quad B \quad 1119.208 \\
C & \quad 8.91170 \quad C \quad 230.738 \\
D & \quad 4.385677 \quad \text{Frost-Kalkwarf equation:} \\
E & \quad 1.054940 \quad \text{derived from exptl. data} \\
\end{align*}

Frost-Kalkwarf equation:

\[
\begin{align*}
A &= 21.62180 \\
B &= -2131.85 \\
C &= 4.83947 \\
D &= 1.41701
\end{align*}
\]

The coefficients are calculated from molecular structures, normal bp and
### TABLE 2.1.1.2.1.2

<table>
<thead>
<tr>
<th>Ashton et al. 1943</th>
<th>Willingham et al. 1945</th>
<th>Stull 1947</th>
<th>Pasek &amp; Thodos 1962</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>static method-manometry</strong></td>
<td><strong>ebulliometry</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>selected experimental data</strong></td>
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<td>( t/°C )</td>
<td>( P/Pa )</td>
<td>( t/°C )</td>
<td>( P/Pa )</td>
</tr>
<tr>
<td>( \Delta H_v/(kJ \text{ mol}^{-1}) = 29.21 )</td>
<td>( )</td>
<td>( )</td>
<td>( )</td>
</tr>
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<td>( )</td>
<td>( )</td>
<td>( )</td>
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</tbody>
</table>

2.

<table>
<thead>
<tr>
<th>Zwolinski &amp; Wilhoit 1971</th>
<th>Mokbel et al. 1995</th>
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<td><strong>selected values</strong></td>
<td><strong>static method-manometry</strong></td>
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<td>( P/Pa )</td>
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<td>( 6666 )</td>
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<td>( 48.453 )</td>
<td>( 98659 )</td>
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<tr>
<td>( 49.262 )</td>
<td>( 101325 )</td>
</tr>
</tbody>
</table>

\( \Delta H_v/(kJ \text{ mol}^{-1}) = \) 28.53 at 25°C  
Wagner eq. given in ref.

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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

<table>
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<tr>
<th>$t/°C$</th>
<th>$H/(kPa \cdot m^3/mol)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>27.9</td>
<td>16.617</td>
</tr>
<tr>
<td>35.8</td>
<td>24.318</td>
</tr>
<tr>
<td>45.0</td>
<td>30.398</td>
</tr>
</tbody>
</table>

$\ln [H/(Pa \cdot m^3/mol)] = A - B/(T/K)$

<table>
<thead>
<tr>
<th>$H/(kPa \cdot m^3/mol)$</th>
<th>$A$</th>
<th>$B$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>14 ± 2.03</td>
<td>3351 ± 633</td>
</tr>
</tbody>
</table>

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: C₆H₁₂
Molecular Weight: 84.159

Melting Point (°C):
-142.42 (Lide 2003)

Boiling Point (°C):
71.8 (Lide 2003)

Density (g/cm³ at 25°C):
0.7487, 0.7439 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm³/mol):
112.4, 113.1 (20°C, 25°C, calculated from density)
121.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
41.59, 29.08 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
6.929 (Riddick et al. 1986)
6.93 (Chickos et al. 1999)

Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
53.01, 43.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
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, Mańczyński et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):

16680 (22.75°C, ebulliometry-manometer, measured range 15.0–22.6°C, Willingham et al. 1945)
\[ \log (P/mmHg) = 6.86283 - 1186.059/(229.042 + t/°C); \text{ temp range } 15.0–22.6°C \] (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
17870 (Antoine eq. regression, temp range –53.7 to 71.8°C, Stull 1947)
18330 (calculated from exptl. determined data, Dreisbach 1955)
\[ \log (P/mmHg) = 6.86283 - 1186.059/(226.042 + t/°C); \text{ temp range } -5 \text{ to } 125°C \] (Antoine eq. for liquid state, Dreisbach 1955)
18302 (interpolated-Antoine eq., temp range –23.7 to 95.7°C, Zwolinski & Wilhoit 1971)
\[ \log (P/mmHg) = 6.86283 - 1186.059/(226.042 + t/°C); \text{ temp range } -23.7 \text{ to } 95.7°C \] (Antoine eq., Zwolinski & Wilhoit 1971)
17850 (interpolated-Antoine eq., temp range –53.7 to 71.8°C, Weast 1972–73)
\[ \log (P/mmHg) = [-0.2185 \times 7490.0/(T/K)] + 7.945471; \text{ temp range } -53.7 \text{ to } 71.8°C \] (Antoine eq., Weast 1972–73)
\[ \log (P/atm) = [1 – 344.830/(T/K)] \times 10^{4\times(0.872156 – 9.88091 \times 10^{-3}\cdot(T/K) + 10.8367 \times 10^{-3}\cdot(T/K)^2)}; \text{ temp range: } 183.15–513.15 K \] (Cox eq., Chao et al. 1983)
log (P/kPa) = 5.99178 – 1188.32/(226.307 + t/°C); temp range 15.035–72.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.86283 – 1186.059/(226.04 + t/°C); temp range –24 to 96°C (Antoine eq., Dean 1985, 1992)

log (P/kPa) = 5.98773 – 1186.059/(226.042 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/kPa) = 5.98551 – 1184.874/(–47.232 + T/K); temp range 288–346 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 32.4766 – 2.6434 × 10³/(T/K) – 8.733·log (T/K) + 2.0749 × 10–11·(T/K) + 3.2158 × 10–6·(T/K)²; temp range 131–533 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

36664 (calculated as 1/K AW, C W/C 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 χ, 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 K OW:

2.35 (calculated-π 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 K OA:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K OC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k OH for reaction with OH radical, k NO₃ with NO₃ radical and k O₃ with O₃ or as indicated, *data at other temperatures see reference:

k OH = 7.10 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ (Atkinson 1990, 1991)

k NO₃ = 7.10 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ with a estimated lifetime τ = 20 h in summer daylight (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k1) and Elimination (k2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric t½ ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

rate constant k = 7.10 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ for the reaction with hydroxyl radical in air (Atkinson 1990, 1991, Altshuller 1991); and an estimated reaction lifetime τ = 20 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: C₈H₁₆
Molecular Weight: 112.213
Melting Point (°C):
-142.4 (Lide 2003)
Boiling Point (°C):
104.9 (Lide 2003)
Density (g/cm³ at 20°C):
0.7483, 0.7430 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
146.0 (20°C, calculated-density, Wang et al. 1992)
166.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
36.23, 32.35 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
3.73 (shake flask-GC, Price 1976)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P/mmHg) = 6.80948 – 1275.998/(219.899 + t°C); temp range 28.9–105.8°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)
5300 (calculated from determined data, Dreisbach 1955)
log (P/mmHg) = 6.80947 – 1275.998/(219.899 + t°C); temp range 20–140°C (interpolated-Antoine eq. for liquid state, Dreisbach 1955)
5300 (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.80947 – 1275.998/(219.899 + t°C); temp range –0.30 to 131.3°C (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.80947 – 1275.998/(219.899 + t°C); temp range 28.944–105.8°C (extrapolated-Antoine eq. from reported expnl. data, Boublik et al. 1984)
log (P/mmHg) = 6.80932 – 1275.928/(219.893 + t°C); temp range 29.0–106°C (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
159000 (calculated-P/C, Mackay & Shiu 1981)
Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.28 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)
- 3.34 (calculated-molar volume $V_M$, Wang et al. 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Air: atmospheric $t_{1/2} \sim 2.4–24$ 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:** C<sub>8</sub>H<sub>16</sub>  
**Molecular Weight:** 112.213  
**Melting Point (°C):**  
-117.3 (Dreisbach 1955; Lide 2003)  
**Boiling Point (°C):**  
130.937 (Willingham et al. 1945)  
131 (Lide 2003)  
**Density (g/cm<sup>3</sup> at 20°C):**  
0.7763, 0.7723 (20°C, 25°C, Dreisbach 1955)  
**Molar Volume (cm<sup>3</sup>/mol):**  
144.6 (20°C, calculated-density)  
166.1 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Vaporization, ΔH<sub>v</sub> (kJ/mol):**  
41.197, 34.746 (25°C, bp, Dreisbach 1955)  
**Enthalpy of Fusion, ΔH<sub>fus</sub> (kJ/mol):**  
10.04 (Chickos et al. 1999)  
**Entropy of Fusion, ΔS<sub>fus</sub> (J/mol K):**  
64.45, 57.9 (exptl., calculated-group additivity method, Chickos et al. 1999)  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m<sup>3</sup> or mg/L at 25°C):**  
2.04 (shake flask-GC, Price 1976)  
1.77 (shake flask-GC, Krzyzanowska & Szeliga 1978)  
**Vapor Pressure (Pa at 25°C and reported temperature dependence equations):**  
\[
\log (P/\text{mmHg}) = 6.98887 - 1380.391/(212.610 + t/°C); \text{temp range 51.7–131.9°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)}
\]
\[
\log (P/\text{mmHg}) = 6.30392 - 1384.386/(213.159 + t/°C); \text{temp range 51.9–131.9°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)}
\]
1650 (calculated by formula, Dreisbach 1955)  
1640 (interpolated-Antoine eq., temp range –21.3 to 158.2°C, Zwolinski & Wilhoit 1971)  
1646 (extrapolated-Antoine eq., Boublík et al. 1973)  
log (P/\text{mmHg}) = 6.91061 - 1388.511/(213.615 + t/°C); temp range 51.88–131.97°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublík et al. 1973)  
1640, 5320 (quoted, calculated-bp, Mackay et al. 1982)  
log (P/\text{atm}) = [1–427.713/(T/K)] × 10^0 \times 0.865420 – 7.04026 × 10^{-4} \times (T/K) + 5.98562 × 10^{-7} \times (T/K)^2; \text{temp range: 313.35–458.95 K (Cox eq., Chao et al. 1983)}
\]
1644 (extrapolated-Antoine eq., temp range 40–186°C, Dean 1985, 1992)  
log (P/\text{mmHg}) = 6.88646 – 1460.80/(207.94 + t/°C); temp range 40–186°C (Antoine eq., Dean 1985, 1992)  
log (P/\text{kPa}) = 6.04236 – 1393.284/(–58.949 + T/K); temp range 323–406 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 33.922 – 3.2097 \times 10^3/(T/K) – 8.9914 \cdot \log(T/K) – 3.2992 \times 10^{-11} \cdot (T/K) + 2.0684 \times 10^{-6} \cdot (T/K)^2; \text{ temp range } 156–603 \text{ K (vapor pressure eq., Yaws 1994)}

Henry’s Law Constant (Pa m^3/mol at 25°C):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>90200</td>
<td>(calculated-P/C, Mackay &amp; Shiu 1981)</td>
</tr>
<tr>
<td>90430</td>
<td>(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)</td>
</tr>
</tbody>
</table>

Octanol/Water Partition Coefficient, log $K_{ow}$:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.95</td>
<td>(calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)</td>
</tr>
<tr>
<td>2.65</td>
<td>(calculated-molar volume $V_M$, Wang et al. 1992)</td>
</tr>
<tr>
<td>4.37</td>
<td>(calculated-fragment const., Müller &amp; Klein 1992)</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{oa}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
2.1.1.2.5 Pentylcyclopentane

Common Name: Pentylcyclopentane
Synonym: 1-cyclopentylpentane
Chemical Name: pentylicyclopentane
CAS Registry No: 3741-00-2
Molecular Formula: C\textsubscript{10}H\textsubscript{20}
Molecular Weight: 140.266
Melting Point (°C): –83 (Dreisbach 1955; Lide 2003)
Boiling Point (°C): 180 (Dreisbach 1955; Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C): 0.7912, 0.7874 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm\textsuperscript{3}/mol): 177.3, 178.1 (20°C, 25°C, calculated-density)
210.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol): 51.12, 39.94 (25°, bp, Dreisbach 1955)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C): 0.115 (shake flask-GC, Price 1976)
0.13 (calculated-recommended liquid-liquid equilibrium LLE data, Ma\c{c}zy\'nski et al. 2004)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations): 159 (calculated by formula, Dreisbach 1959)
\[\log (P/\text{mmHg}) = 6.929 – 1526.0/(197.0 + t/°C); \text{ temp range } 85–220°C \] (Antoine eq. for liquid state, Dreisbach 1955)
152 (extrapolated-Antoine eq., temp range 60–210°C, Zwolinski & Wilhoit 1971)
\[\log (P/\text{mmHg}) = 6.9414 – 1540.6/(198.8 + t/°C); \text{ temp range } 60–210°C \] (Antoine eq., Zwolinski & Wilhoit 1971)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C): 18500 (calculated-P/C, Mackay & Shiu 1981)
18600 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\):
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log \(K_{\text{OC}}\):
Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_\text{1/2}\):
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: C₆H₁₂
Molecular Weight: 84.159

Melting Point (°C):
6.59  (Lide 2003)

Boiling Point (°C):
80.73  (Lide 2003)

Density (g/cm³ at 20°C):
0.7786, 0.7739  (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm³/mol):
108.1  (20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981)
118.2  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆HV (kJ/mol):
32.89, 30.05  (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ∆Hₙ (kJ/mol):
2.677  (Riddick et al. 1986)
5.84, 2.68; 9.41  (~87.05, 6.65°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ∆Sₙ (J/mol K):
45.77, 44.55  (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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*  (shake flask-GC/FID, measured range 5.11–45.21°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  (23.5°C, elution chromatography, Schwarz 1980)
72.4  (calculated-HPLC-k² correlation, converted from reported γₒ, Hafkenscheid & Tomlinson 1983)
72.8*  (40°C, shake flask-GC, measured range 40–209.06°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/(T/K) + 43.2980·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 2001)
ln x = –219.863 + 6693.78/(T/K) + 31.3744·ln (T/K); temp range 290–400 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, Mačzyński et al. 2004)

Vapor Pressure (Pa at 25°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*  (30°C, vapor-liquid equilibrium VLE data, measured range 30–80°C, Scatchard et al. 1939)
\[ \log (P/\text{mmHg}) = 6.65859 - 104.0641/(T/K) - 104.865/(T/K)^2; \text{ temp range 30–60}^\circ\text{C (VLE data, Scatchard et al. 1939)} \]

10910* (20.97°C, manometry, measured range 6.33–20.97°C, Aston et al. 1943b)

11700* (20.96°C, ebulliometry-manometer, measured range 19.9–81.6°C, Willingham et al. 1945)

\[ \log (P/\text{mmHg}) = 6.84498 - 120.3526/(222.863 + t/°C); \text{ temp range 19.9–81.6°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)} \]

12280* (calculated-Antoine eq. regression, temp range –45.3 to 80.7°C, Stull 1947)

10253*; 10375 (20.015°C, selected exptl., calculated-Frost-Kalkwarf vapor pressure eq., temp range 293.185–551.225 K, Pasek & Thodos 1962)

\[ \log (P/\text{mmHg}) = 6.84498 - 1203.526/(222.863 + t/°C); \text{ temp range 19.9–81.6°C (Antoine eq. for liquid state, Dreisbach 1955)} \]


\[ \log (P/\text{mmHg}) = 6.84130 - 1201.531/(222.65 + t/°C); \text{ temp range 20–81°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]

11170 (interpolated-Antoine eq., temp range –45.3 to 257.5°C, Weast 1972–73)

\[ \log (P/\text{mmHg}) = [-0.2185 × 7830.9/(T/K)] + 7.662126; \text{ temp range –45.3 to 257.5°C (Antoine eq., Weast 1972–73)} \]

\[ \log (P/\text{atm}) = [1 – 353.663/(T/K)] × 10^{0.881199 – 9.58655 × 10^{-4·(T/K) + 9.72305 × 10^{-7·(T/K)^2}}}; \text{ temp range 227.85–553.64 K (Cox eq., Chao et al. 1983)} \]

13010, 13040 (interpolated-Antoine equations, Boublik et al. 1984)

\[ \log (P/\text{kPa}) = 5.97561 – 1206.731/(223.223 + t/°C); \text{ temp range 19.9–81.6°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)} \]

\[ \log (P/\text{kPa}) = 6.98226 – 1211.248/(223.869 + t/°C); \text{ temp range 25–75°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]

\[ \log (P/\text{kPa}) = 6.00569 – 1223.273/(225.089 + t/°C); \text{ temp range 17.55–80.22°C (Antoine eq. from reported exptl. data of Cruickshank & Cutler 1967, Boublik et al. 1984)} \]

13020 (interpolated-Antoine eq., temp range 20–81°C, Dean 1985, 1992)

\[ \log (P/\text{mmHg}) = 6.84130 – 1201.531/(222.65 + t/°C); \text{ temp range 20–81°C (Antoine eq., Dean 1985, 1992)} \]

13040 (lit. average, Riddick et al. 1986)

\[ \log (P/\text{kPa}) = 5.96407 – 1200.31/(222.504 +t/°C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)} \]

13070 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

\[ \log (P/\text{kPa}) = 7.2778 – 1747.2/(26.84 + T/K); \text{ temp range 223–280 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)} \]

\[ \log (P/\text{kPa}) = 5.9682 – 1201.531/(–50.503 + T/K); \text{ temp range 293–335 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]

\[ \log (P/\text{kPa}) = 6.03245 – 1244.124/(–44.911 + T/K); \text{ temp range 353–414 K (Antoine eq.-III, Stephenson & Malanowski 1987)} \]

\[ \log (P/\text{kPa}) = 6.36849 – 1519.732/(–4.032 + T/K); \text{ temp range 412–491 K (Antoine eq.-IV, Stephenson & Malanowski 1987)} \]

\[ \log (P/\text{kPa}) = 7.37347 – 2683.075/(159.31 + T/K); \text{ temp range 489–533 K (Antoine eq.-V, Stephenson & Malanowski 1987)} \]

12920, 1730 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

\[ \log (P/\text{mmHg}) = 48.5529 – 3.0874 × 10^{10/(T/K)} – 15.521\log (T/K) + 7.383 × 10^{-3·(T/K)} + 6.3563 × 10^{-12·(T/K)^2}; \text{ temp range 280–554 K (vapor pressure eq., Yaws 1994)} \]


16230, 36180 (30, 50°C, VLE equilibrium data, Carmona et al. 2000)
Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

<table>
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<tr>
<th>Value</th>
<th>Source</th>
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<td>19860</td>
<td>(calculated-P/C, Mackay &amp; Shiu 1975)</td>
</tr>
<tr>
<td>19690</td>
<td>(calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine &amp; Mookerjee 1975)</td>
</tr>
<tr>
<td>18380, 27810</td>
<td>(calculated-group contribution, calculated-bond contribution, Hine &amp; Mookerjee 1975)</td>
</tr>
<tr>
<td>18000</td>
<td>(recommended; Mackay &amp; Shiu 1981)</td>
</tr>
<tr>
<td>22092</td>
<td>(calculated-MCI  \chi, Nirmalakhandan &amp; Speece 1988)</td>
</tr>
<tr>
<td>17935*</td>
<td>(EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)</td>
</tr>
<tr>
<td>5532, 17935,19353, 1450</td>
<td>(bubble column non-equilibrium measurement, EPICS-GC, direct concentration. ratio, calculated-UNIFAC activity coeff., Ashworth et al. 1988)</td>
</tr>
<tr>
<td>37190*</td>
<td>(40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)</td>
</tr>
<tr>
<td>15062</td>
<td>(20°C, selected from reported experimental determined values, Staudinger &amp; Roberts 1996, 2001)</td>
</tr>
</tbody>
</table>

\[ \ln \frac{[H]}{(\text{atm} \cdot \text{m}^3/\text{mol})} = 9.141 – 3238/(T/\text{K}); \text{temp range: 10–30°C} \] (EPICS measurements, Ashworth et al. 1988)

Octanol/Water Partition Coefficient, log K_{OW}:

- 2.46 (calculated-\pi substituent constant, Hansch et al. 1968)
- 3.44 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)
- 3.40 (Cramer 1977)
- 3.18, 3.48, 3.48 (calculated-fragment const., Rekker 1977)
- 3.69 (HPLC-k’ correlation, Hafkenscheid & Tomlinson 1983)
- 3.70 (from activity coefficient measurement, Bertl et al. 1986)
- 3.44 (recommended, Sangster 1989, 1993)
- 3.73 (from activity coefficient measurement, Tse & Sandler 1994)
- 3.44 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated. Additional data at other temperatures designated* are compiled at the end of this section:

- 2.83* (20.29°C, from GC-determined \gamma in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
- 2.71 (calculated-measured \gamma in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 2.38 (estimated, Howard 1990)

Sorption Partition Coefficient, log K_{OC}:

- 2.68 (estimated-S, Howard 1990)

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:

- Volatilization: t_1/2 = 2.8 h from a model river 1 m deep with a 1 m/s current and a 3 m/s wind (Lyman et al. 1982, quoted, Howard 1990).
- Photolysis:
  - Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
    - k_{OH} (exptl) = 5.38 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}, k_{OH} (calc) = 4.79 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} at 295 K, measured range 295–497 K (flash photolysis-kinetic spectroscopy, Greiner 1970)
    - k_{OH} (exptl) = 6.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at 298 K; k_{OH} (calc) = 6.7 \times 10^{-12} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} at 300 K (Darnall et al. 1978)
    - k_{O(3P)} = 1.40 \times 10^{-13} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} for the reaction with O(3P) atoms at room temp. (Herron & Huie 1973)
    - k_{OH} = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at room temp. (Atkinson et al. 1979)
    - k_{OH} = (7.57 \pm 0.05) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} at room temp. (relative rate, Atkinson et al. 1984c)
$k_{OH} = (6.20 \pm 0.44) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at $(24.4 \pm 0.4)^\circ$C with an atmospheric lifetime of 1.9 d for an average OH radical concentration of $1.0 \times 10^6$ molecules/cm$^3$ (Edney et al. 1986)

$k_{OH} = 7.34 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 K (Atkinson 1986; quoted, Edney et al. 1986)

$k_{OH} = 7.14 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 292 K, measured range 292–491 K (Droegge & Tully 1987)

$k_{OH} = 7.38 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Dilling et al. 1988)

$k_{OH} = 7.49 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 7.49 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, $k_{NO_3} = 13.4 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson 1990)

$k_{NO_3} = 1.35 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson 1991)

$k_{NO_3}(exp) = 1.35 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO_3}(calc) = 2.04 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 $\pm$ 2 K (relative rate method, Aschmann & Atkinson 1995)

$k_{OH}^* = 7.21 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO_3} = 1.4 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

$k_{OH}^* = 6.69 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 230–400 K (relative rate method, DeMore & Bayes 1999)

**Hydrolysis:**

Biodegradation: highly resistant to biodegradation (Howard 1990);

$\tau_{aq. aerobic} = 672$ to 4032 h, based on unacclimated grab sample of aerobic soil and aerobic aqueous screening test data (Howard et al. 1991);

$\tau_{aq. anaerobic} = 2688$ to 16280 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

**Biotransformation:**

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

**Half-Lives in the Environment:**

Air: atmospheric $\tau = 2.4$–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (Darnall et al. 1976);

atmospheric lifetime $\tau = 1.9$ d for an average OH radical concentration of $1.0 \times 10^6$ molecules/cm$^3$ (Edney et al. 1986);

$\tau_{aq. aerobic} = 52$ h, based on photooxidation rate constant (Howard 1990);

an atmospheric lifetime $\tau = 19$ h in summer daylight, based on the photooxidation reaction rate constant of $7.49 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction with OH radical in air during summer daylight (Altshuller 1991);

will degrade photochemically by hydroxyl radicals with $\tau_{aq. aerobic} = 52$ h and much faster under photochemical smog conditions with $\tau_{aq. aerobic} = 6$ h (Howard 1990);

$\tau_{aq. aerobic} = 8.7$–87 h, based on reaction with OH radical half-life in air (Howard et al. 1991).

Surface water: volatilization $\tau_{aq. aerobic} = 2$ h in a model river (Howard 1990);

$\tau_{aq. aerobic} = 672$ to 4320 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

photooxidation $\tau_{aq. aerobic} = 1.4 \times 10^9$ to $6.9 \times 10^{10}$ h (16000 to 780000 yr), based on measured rate data for alkylperoxyl radicals in aqueous solution (Howard et al. 1991).

Ground water: $\tau_{aq. aerobic} = 1344$–8640 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $\tau_{aq. aerobic} = 672$–4320 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

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<th>Tsonopoulos &amp; Wilson 1983</th>
<th>Shaw 1989a</th>
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<td></td>
<td>shake flask-GC</td>
<td>IUPAC recommended</td>
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<td><strong>S/g·m⁻³</strong></td>
<td><strong>t/°C</strong></td>
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<tr>
<td>5.11</td>
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<td>15.21</td>
<td>88.70</td>
<td>100</td>
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<td>35.21</td>
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<td>45.21</td>
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<td>209.06</td>
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**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:

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) + D \cdot P/(T/K)^2 \quad (5) \\
\log P &= A - B/T(T/K) - C/(T/K)^2 \quad (6)
\end{align*}
\]

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<tr>
<th>Ashton et al. 1943b</th>
<th>Willingham et al. 1945</th>
<th>Stull 1947</th>
<th>Pasek &amp; Thodos 1962</th>
</tr>
</thead>
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<td>ebuliometry</td>
<td>summary of literature data</td>
<td>selected exptl. data</td>
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<td>20.97</td>
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<td>34.821</td>
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\[
\Delta H_v/(kJ \cdot mol^{-1}) = 33.33 \quad (at 25°C)
\]

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<th>Scatchard et al. 1939</th>
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<td>24613</td>
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<td>36237</td>
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(Continued)
2.  

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<td>15109</td>
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<td>50.96</td>
<td>37543</td>
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<td>56.18</td>
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<td>49.393</td>
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<td>62.46</td>
<td>56448</td>
<td>∆HV/(kJ mol⁻¹) =</td>
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<td>79993</td>
<td>55.302</td>
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<tr>
<td>68.71</td>
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<td>33.23</td>
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<td>75.42</td>
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<td>78.944</td>
<td>95992</td>
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<td>54.1°C</td>
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<tr>
<td>eq. 2</td>
<td>P/mmHg</td>
<td>eq. 2</td>
<td>P/mmHg</td>
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<tr>
<td>A</td>
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<td>6.84130</td>
<td>87.149</td>
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<tr>
<td>B</td>
<td>1212.014</td>
<td>B</td>
<td>1201.531</td>
<td>data fitted to Wagner eq.</td>
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<tr>
<td>C</td>
<td>233.956</td>
<td>C</td>
<td>222.647</td>
<td>80.732</td>
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</tr>
<tr>
<td>∆HV/(kJ mol⁻¹) =</td>
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<td>33.04</td>
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<tr>
<td>at bp</td>
<td>29.96</td>
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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

$\ln K_{AW} = A - B/(T/K)$  \hspace{1cm}  (1)
$\log K_{AW} = A - B/(T/K)$  \hspace{1cm}  (1a)
$\ln (1/K_{AW}) = A - B/(T/K)$  \hspace{1cm}  (2)
$\log (1/K_{AW}) = A - B/(T/K)$  \hspace{1cm}  (2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$  \hspace{1cm}  (3)
$\ln \left[ H/(\text{Pa m}^3/\text{mol}) \right] = A - B/(T/K)$  \hspace{1cm}  (4)
$K_{AW} = A - B/\left(T/K\right) + C*\left(T/K\right)^2$  \hspace{1cm}  (5)

Henry’s law constant

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<td>EPICS-GC</td>
<td>equilibrium headspace-GC</td>
<td>GC det'd activity coefficient</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m^3/mol)</td>
<td>t/°C</td>
</tr>
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<td>10436</td>
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<tr>
<td>15</td>
<td>12767</td>
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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 $K_{OA}$ versus reciprocal temperature for cyclohexane.
Common Name: Methylcyclohexane
Synonym: hexahydrotoluene, cyclohexylmethane
Chemical Name: methylcyclohexane
CAS Registry No: 108-87-2
Molecular Formula: C\textsubscript{7}H\textsubscript{14}
Molecular Weight: 98.186
Melting Point (°C):
-126.6 (Dreisbach 1959; Weast 1984; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
100.93 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.7694, 0.7651 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)
Molar Volume (cm\textsuperscript{3}/mol):
127.6 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
140.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
35.359, 31.13 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
6.757, 6.75 (Riddick et al. 1986)
6.75 (Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
46.1, 47.3 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°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°C, Price 1976; quoted, Eastcott et al. 1988)
15.3 (partition coefficient-GC, Rudakov & Lutsyk 1979)
15.2 (20°C, shake flask-GC, Burris & MacIntyre 1986)
16.7 (shake flask-GC, Groves 1988)
15.1* (IUPAC recommended, temp range 25–150°C, Shaw 1989)
15.82* (calculated-liquid-liquid equilibrium LLE data, temp range 298.2–410.5 K, Mączyński et al. 2004)
ln (S/ppm) = 13.091 – 7085.522/(T/K) + 1055594/(T/K)\textsuperscript{2} (Marche et al. 2004)

Vapor Pressure (Pa at 25°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 (P/mmHg) = 6.95423 – 1336.93/(T/K – 45.52); temp range 4–75°C (Antoine eq. based on exptl. data, Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)
6354* (25.59°C, ebulliometry-manometer, Willingham et al. 1945)
log (P/mmHg) = 6.82689 – 1272.864/(221.630 + t°C); temp range 25.6–101.8°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)
5887* (calculated-Antoine eq. regression, temp range –35.9 to 100.0°C, Stull 1947)
6180 (calculated from determined data, Dreisbach 1955)
log (P/mmHg) = 6.82689 – 1272.864/(221.630 + t°C); temp range 10–155°C (Antoine eq. for liquid state, Dreisbach 1955)
10207* (35.901°C, temp range 35.901–95.946°C, Varushchenko et al. 1970)
log (P/mmHg) = 6.82300 – 1272.763/(221.42 + t/°C); temp range –3 to 127°C (Antoine eq., Dean 1985, 1992)

Henry’s Law Constant (Pa m3/mol at 25°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/KAW, Cw/Cv, reported as exp., Hine & Mookerjee 1975)
31030, 41340 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
40000 (recommended; Mackay & Shiu 1981)
31934 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
37930 (calculated-P/C, Eastcott et al. 1988)
43300 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log KOW:

2.76 (calculated-π substituent constant, Hansch et al. 1968)
2.96 (calculated- MCI π, 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 Vm, Wang et al. 1992)
3.87  (calculated-fragment const., Müller & Klein 1992)
3.61  (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.14*  (20.29°C, from GC-determined $\gamma^\infty$ in octanol, measured range 20.29–50.28°C Gruber et al. 1997)
3.05  (calculated-measured $\gamma^\infty$ in pure octanol and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH} = (10.6 \pm 0.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (relative rate, Atkinson et al. 1984c)

$k_{OH} = 1.04 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = 1.04 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K with an estimated half-life of 13 h (Altshuller 1991)

$k_{OH} = 1.0 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biotransformation:

Biodegradation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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 $1.04 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with hydroxyl radicals in air (Altshuller 1991).

### TABLE 2.1.1.2.7.1
Reported aqueous solubilities of methylcyclohexane at various temperatures

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<thead>
<tr>
<th></th>
<th></th>
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<tbody>
<tr>
<td><strong>Shake flask-GC</strong></td>
<td><strong>IUPAC recommended</strong></td>
<td><strong>Shake flask-GC</strong></td>
<td><strong>Calc-recommended LLE data</strong></td>
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<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
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<tr>
<td>25.0</td>
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<td>149.5</td>
<td>244</td>
<td>110</td>
<td>52.0</td>
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$S = A - B/(T/K) + C/(T/K)^2$

<table>
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<tr>
<th>$S$</th>
<th>$g/m^3$</th>
<th>$A$</th>
<th>$B$</th>
<th>$C$</th>
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<tr>
<td>13.091</td>
<td>7085.522</td>
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</table>
**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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\ln P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\ln P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\ln P &= A - B/(C + T/K) - C \cdot \log (T/K) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) + D\left[\frac{P}{(T/K)^2}\right]
\end{align*}
\]

1. **Willingham et al. 1945**

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(P/Pa)</th>
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<td>25.585</td>
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<tr>
<td>29.533</td>
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<td>42.929</td>
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**Stull 1947**

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**Varushchenko et al. 1970**

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**Zwolinski & Wilhoit 1971**

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<td>P/Pa</td>
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<td>100.715</td>
<td>100697</td>
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<td>101.312</td>
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<tr>
<td>101.832</td>
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bp/°C: 100.934

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<td>B</td>
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<tr>
<td>C</td>
<td>221.630</td>
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</table>

∆HV/(kJ mol–1) =

- at 25°C 35.36
- at bp 31.13

### 2.

#### Mokbel et al. 1995

<table>
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<tr>
<td>t/°C</td>
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<td>–48.64</td>
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<td>–38.15</td>
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Methylcyclohexane: vapor pressure vs. 1/T

**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

\[ \ln K_{AW} = A - \frac{B}{T/K} \]  
(1)  
\[ \log K_{AW} = A - \frac{B}{T/K} \]  
(1a)  
\[ \ln \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} \]  
(2)  
\[ \log \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} \]  
(2a)  
\[ \ln \left( \frac{\text{H/(Pa m}^3\text{/mol)}}{\text{atm}} \right) = A - \frac{B}{T/K} \]  
(3)  
\[ \ln \left( \frac{\text{H/(Pa m}^3\text{/mol)}}{\text{atm} \cdot \text{m}^3\text{/mol}} \right) = A - \frac{B}{T/K} \]  
(4)  
\[ \ln \left( \frac{\text{H/(Pa m}^3\text{/mol)}}{\text{atm} \cdot \text{m}^3\text{/mol}} \right) = A - \frac{B}{T/K} \]  
(4a)  
\[ K_{AW} = A - \frac{B}{T} + C \left( \frac{T}{K} \right)^2 \]  
(5)  

Henry's law constant

<table>
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</tr>
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<tbody>
<tr>
<td><strong>EPICS-GC</strong></td>
<td><strong>GC det'd activity coefficient</strong></td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(kPa m³/mol)</strong></td>
</tr>
<tr>
<td>27.3</td>
<td>12.666</td>
</tr>
<tr>
<td>35.8</td>
<td>34.653</td>
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<tr>
<td>45.0</td>
<td>72.447</td>
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</table>

\[ \text{eq. 4} \] \[ H/(\text{kPa m}^3\text{/mol}) \]
A 34 ± 3.39  
B 9406 ± 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 $K_{OA}$ versus reciprocal temperature for methylcyclohexane.
2.1.1.2.8 1,2-\textit{cis}-Dimethylcyclohexane

Common Name: 1,2-\textit{cis}-Dimethylcyclohexane
Synonym: \textit{cis}-1,2-dimethylcyclohexane
Chemical Name: 1,2-\textit{cis}-dimethylcyclohexane
CAS Registry No: 2207-01-4
Molecular Formula: C\textsubscript{8}H\textsubscript{16}
Molecular Weight: 112.213

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<th>Property</th>
<th>Value</th>
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<td>Melting Point (°C)</td>
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</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>129.8 (Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm\textsuperscript{3} at 20°C)</td>
<td>0.7963, 0.7922 (20°C, 25°C, Dreisbach 1955; Riddick et al. 1986)</td>
</tr>
<tr>
<td>Molar Volume (cm\textsuperscript{3}/mol)</td>
<td>140.9 (20°C, calculated-density, McAuliffe 1966)</td>
</tr>
<tr>
<td></td>
<td>141.6 (25°C, calculated-density; Ruelle &amp; Kesselring 1997)</td>
</tr>
<tr>
<td></td>
<td>162.6 (calculated-Le Bas method at normal boiling point)</td>
</tr>
<tr>
<td>Enthalpy of Vaporization, (\Delta H_v) (kJ/mol)</td>
<td>39.715, 34.196 (25°C, bp, Riddick et al. 1986)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, (\Delta H_{ fus}) (kJ/mol)</td>
<td>1.644 (Dreisbach 1955; Riddick et al. 1986)</td>
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<tr>
<td></td>
<td>8.26, 1.64 (--100.65, –39.05°C, Chickos et al. 1999)</td>
</tr>
<tr>
<td>Entropy of Fusion, (\Delta S_{ fus}) (J/mol K)</td>
<td>55.22, 50.2 (exppl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)</td>
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<td>Fugacity Ratio at 25°C, F</td>
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Water Solubility (g/m\textsuperscript{3} or mg/L at 25°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, Mączynski et al. 2004)  
5.94* (generator column-GC, measured range 273.15–313.15 K, Dohányosová et al. 2004)  
\[\ln x = -59.7348 + 45.8700/\tau + 46.6282\cdot\ln \tau; \tau = T/298.15 \text{ K} \] (empirical eq., generator column-GC, Dohányosová et al. 2004)  
\[\ln (S/ppm) = 11.610 – 8455.943/(T/K) + 961943.2/(T/K)^2, \text{ temp range 30.3–170°C} \] (Marche et al. 2004)  

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):  
6352* (49.185°C, ebulliometry, measured range 49.185–130.684°C, Willingham et al. 1945)  
1333* (18.4°C, summary of literature data, temp range –15.9 to 129.7°C, Stull 1947)  
\[\log (P/mmHg) = 6.84164 – 1369.525/(216.040 + t/°C); \text{ temp range 49.2–130.7°C} \] (Antoine eq. from exppl. data, ebulliometry-manometer, Willingham et al. 1945)  
1929 (calculated by formula, Dreisbach 1955)  
\[\log (P/mmHg) = 6.84164 – 1369.525/(216.040 + t/°C); \text{ temp range 40–170°C} \] (Antoine eq. for liquid state, Dreisbach 1955)  
1933* (interpolated-Antoine eq., temp range 18.4–157.6°C, Zwolinski & Wilhoit 1971)  
\[\log (P/mmHg) = 6.83746 – 1367.311/(215.835 + t/°C); \text{ temp range 18.4–157.6°C} \] (Antoine eq., Zwolinski & Wilhoit 1971)  
\[\log (P/mmHg) = [-0.2185 \times 9364.9/(T/K)] + 8.001159; \text{ temp range –15.9 to 129.7°C} \] (Antoine eq., Weast 1972–73)
Aliphatic and Cyclic Hydrocarbons

\[
\log(\text{P/atm}) = [1-402.894/(\text{T/K})] \times 10^4\{0.841813 - 8.56119 \times 10^{-4}\cdot(\text{T/K}) + 5.01855 \times 10^{-7}\cdot(\text{T/K})^2\}; \text{ temp range: 257.25–430.75 K (Cox eq., Chao et al. 1983)}
\]

1927 (extrapolated-Antoine eq., Boublík et al. 1984)

\[
\log(\text{P/kPa}) = 5.96885 - 1370.962/(216.202 + t/°C); \text{ temp range 49.2–130.68°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublík et al. 1984)}
\]

1928 (interpolated-Antoine eq., temp range 18–158°C, Dean 1985, 1992)

\[
\log(\text{P/mmHg}) = 6.83746 - 1367.311/(215.84 + t/°C); \text{ temp range 18–158°C (Antoine eq., Dean 1985, 1992)}
\]

1928 (interpolated-Antoine eq., temp range 18–158°C, Dean 1985, 1992)

\[
\log(\text{P/kPa}) = 5.96654 - 1369.525/(216.040 + t/°C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

\[
\log(\text{P/mmHg}) = 32.1535 - 3.0728 \times 10^3/(\text{T/K}) - 8.4344\cdot\log(\text{T/K}) + 6.8943 \times 10^{-10}\cdot(\text{T/K}) + 1.9558 \times 10^{-6}\cdot(\text{T/K})^2; \text{ temp range 223–606 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

36000 (calculated-P/C, Mackay & Shiu 1981)
35830 (calculated-1/K_{AW}, C_w/C_A, reported as exptl., Hine & Mookerjee 1975)
53000, 62270 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
44080 (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 K_{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 V_M, Wang et al. 1992)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_0:

Half-Lives in the Environment:

Air: atmospheric t_0 ~ 2.4–24 h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).

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<tr>
<th>T/K</th>
<th>S/g·m⁻³</th>
<th>T/K</th>
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**FIGURE 2.1.1.2.8.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1,2-cis-dimethylcyclohexane.
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

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(Continued)
### TABLE 2.1.1.2.8.2 (Continued)

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<th>Zwolinski &amp; Wilhoit 1971</th>
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<td>pressure range 48–780 mmHg</td>
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**FIGURE 2.1.1.2.8.3** Logarithm of vapor pressure versus reciprocal temperature for 1,2-cis-dimethylcyclohexane.
2.1.1.2.9 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: C$_8$H$_{16}$
Molecular Weight: 112.213
Melting Point (°C): 
-36.93  (Lide 2003)
Boiling Point (°C): 
119.4  (Lide 2003)
Density (g/cm$^3$ at 20°C): 
0.7626, 0.7584  (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm$^3$/mol): 
147.2, 148  (20°C, 25°C, calculated-density)
162.6  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta$H$_v$ (kJ/mol): 
38.14, 33.05  (25°, bp, Dreisbach 1955)
Enthalpy of Fusion, $\Delta$H$_{fus}$ (kJ/mol): 
11.422  (Dreisbach 1955)
12.34  (Chickos et al. 1999)
Entropy of Fusion, $\Delta$S$_{fus}$ (J/mol K): 
52.26, 50.2  (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m$^3$ or mg/L at 25°C): 
3.84  (shake flask-GC, Price 1976; quoted, Shaw 1989)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

\[ \log (P\text{mmHg}) = 6.82180 - 1332.613/(218.791 + t/°C); \text{ temp range 40.3–120.3°C (Antoine eq. from exptl. data, ebulliometry-manometer, Willingham et al. 1945)} \]
3025  (calculated by formula. Dreisbach 1955)
\[ \log (P\text{mmHg}) = 6.82180 - 1332.613/(218.791 + t/°C); \text{ temp range 30–155°C (Antoine eq. for liquid state, Dreisbach 1955)} \]
3026  (interpolated-Antoine eq., temp range 10.1–146.8°C, Zwolinski & Wilhoit 1971)
\[ \log (P\text{mmHg}) = 6.81773 - 1330.437/(218.581 + t/°C); \text{ temp range 10.1–146.8°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]
\[ \log (P\text{mmHg}) = [-0.2185 \times 8951.2/(T/K)] + 7.898079; \text{ temp range –24.3 to 119.5°C (Antoine eq., Weast 1972–73)} \]
\[ \log (P\text{atm}) = [1 – 396.346/(T/K)] \times 10^3\{0.827486 – 6.12608 \times 10^{-4}·(T/K) + 4.53086 \times 10^{-7}·(T/K)^2\}; \text{ temp range: 252.05–424.25 K (Cox eq., Chao et al. 1983)} \]
3024  (interpolated-Antoine eq., temp range 10–147°C, Dean 1985, 1992)
\[ \log (P\text{mmHg}) = 6.81773 – 1330.437/(218.58 + t/°C); \text{ temp range 10–147°C (Antoine eq., Dean 1985, 1992)} \]
\[ \log (P\text{atm}) = 5.94449 – 1331.612/(–54.43 + T/K); \text{ temp range 313–395 K (Antoine eq., Stephenson & Malanowski 1987)} \]
\[ \log (P\text{mmHg}) = 32.5731 – 2.9872 \times 10^3/(T/K) – 8.6494·log (T/K) – 2.1355 \times 10^{-9}·(T/K) + 2.2946 \times 10^{-6}·(T/K)^2; \text{ temp range 236–590 K (vapor pressure eq., Yaws 1994)} \]
Henry’s Law Constant (Pa m³/mol at 25°C):

88200 (calculated-P/C, Mackay & Shiu 1981)
88360 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log $K_{OW}$:

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:

Air: atmospheric $t_\text{½} \approx 2.4$–24 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: C9H18  
Molecular Weight: 126.239  
Melting Point (°C):  
–65.7  (Lide 2003)  
Boiling Point (°C):  
136.6  (Lide 2003)  
Density (g/cm³ at 20°C): 0.7664  
Molar Volume (cm³/mol):  
164.7  (20°C, calculated-density, Ruelle & Kesselring 1997)  
184.8  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):  
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m³ or mg/L at 25°C):  
1.77  (shake flask-GC, Price 1976)  
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):  
$\log (P/\text{mmHg}) = 6.83705 - 1393.299/(215.551 + t/°C)$; temp range 54.7–137.6°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1949)  
$\log (P/\text{atm}) = [1 - 409.802/(T/K)] \times 10^{0.838270 - 6.63916 \times 10^{-4}(T/K) + 5.61172 \times 10^{-7}(T/K)^2}$; temp range: 327.82–410.80 K (Cox eq., Chao et al. 1983)  
1480  (extrapolated-Antoine eq., Boublik et al. 1984)  
$\log (P/\text{kPa}) = 5.96492 - 1395.206/(215.77 + t/°C)$; temp range 54.67–137.7°C (Antoine eq. from reported expctl. data of Forziati et al. 1949, Boublik et al. 1984)  
$\log (P/\text{kPa}) = 5.96816 - 1397.161/(215.961 + t/°C)$; temp range 54.69–137.65°C (Antoine eq. from reported expctl. data of Pasek & Thodos 1962, Boublik et al. 1984)  
1480  (interpolated-Antoine eq., temp range 55–137°C, Dean 1985, 1992)  
$\log (P/\text{mmHg}) = 6.83951 - 1394.88/(215.73 + t/°C)$; temp range 55–137°C (Antoine eq., Dean 1985, 1992)  
$log (P_{L}/\text{kPa}) = 5.96449 - 1395.396/(-57.308 + T/K)$; temp range 348–411 K (Antoine eq., Stephenson & Malanowski 1987)  
Henry’s Law Constant (Pa m³/mol at 25°C):  
105600  (calculated-P/C from selected data)
Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$ for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH} = 8.73 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (Atkinson 1989)

$k_{OH} = 8.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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: C₈H₁₆, C₂H₅C₆H₁₁
Molecular Weight: 112.213
Melting Point (°C): –111.3 (Weast 1982–83; Lide 2003)
Boiling Point (°C): 131.9 (Lide 2003)
Density (g/cm³): 0.7880 (20°C, Weast 1982–82)
Molar Volume (cm³/mol): 142.4 (20°C, calculated-density, Stephenson & Malanowski 1987)
162.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Sublimation, \( \Delta H_{sub} \) (kJ/mol):
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{fus} = 56 \) J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°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* (40°C, shake flask-solid phase extraction-GC, measured range 38.35–280°C, Heidman et al. 1985)
\[ \ln x = -334.2468 + 14105.21/(T/K) + 47.93102 \cdot \ln (T/K); \text{ measured range } 40–280°C \text{ (shake flask-solid phase extraction-GC, Heidman et al. 1985)} \]
7.0* (40°C, IUPAC tentative value, temp range 40–280°C, Shaw 1989a)
3.89* (generator column-GC/FID, measured range 273.15–313.15 K, Dohányosová et al. 2004)
\[ \ln x = -53.6687 + 39.4055/\tau + 41.1210 \cdot \ln \tau, \tau = [(T/K)/298.15], \text{ temp range } 273.15–313.15 K \text{ (generator column-GC/FID, Dohányosová et al. 2004)} \]
4.36* (30.3°C, shake flask-GC, measured range 30.3–170.8°C, Marche et al. 2004)
\[ \ln x = -344.02468 + 14105.21/(T/K) + 47.93102 \cdot \ln (T/K); \text{ temp range } 30.3–170.8°C \text{ (Marche et al. 2004)} \]

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

6351* (51.412°C, ebulliometry, measured range 51.4–132.7°C, Willingham et al. 1945)
1612 (extrapolated-Antoine eq., Willingham et al. 1945)
\[ \log \left( \frac{P}{\text{mmHg}} \right) = 6.87041 – 1384.036/(214.128 + t/°C); \text{ temp range } 51.4–132.7°C \text{ (Antoine eq., ebulliometry, Willingham et al. 1945)} \]
1333* (20.6°C, summary of literature data, temp range –14.5 to 131.9°C, Stull 1947)
1705* (extrapolated-Antoine eq., temp range 20.6–159.5°C, Zwolinski & Wilhoit 1971)
\[ \log \left( \frac{P}{\text{mmHg}} \right) = 6.86728 – 1382.466/(214.995 + t/°C); \text{ temp range } 20.6–159.5°C \text{ (Antoine eq., Zwolinski & Wilhoit 1971)} \]
\[ \log \left( \frac{P}{\text{KPa}} \right) = 5.99043 – 1381.396/(–58.271 + T/K); \text{ temp range } 323–407 K \text{ (Antoine eq., Stephenson & Malanowski 1987)} \]
Henry’s Law Constant (Pa m^3/mol at 25°C Additional data at other temperatures designated * are compiled at the end of this section):

\[
\ln \left( \frac{k_H}{\text{MPa}} \right) = 325.570 - \frac{18496.5}{(T/K)} - 10.9666 \cdot (T/K)^2 - 44.7690 \cdot \ln (T/K); \quad \text{maximum } k_H = 1.186 \times 10^4 \text{ MPa at } 385.2 \text{ K (Heidman et al. 1985)}
\]

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 K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_b:

Sorption Partition Coefficient, log K_{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

\[ \ln x = A + B/(T/K) + C \ln (T/K) \]  

<table>
<thead>
<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
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<td>38.35</td>
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<td>274.15</td>
<td>3.803</td>
<td>30.3</td>
<td>4.358</td>
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<td>94.45</td>
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<td>50</td>
<td>7.0</td>
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<td>55</td>
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<td>B</td>
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<td>550</td>
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</table>

\[
\ln x = A + B/\tau + C \ln \tau
\]

\[
\tau = (T/K)/298.15
\]

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 ethylcyclonexane.

TABLE 2.1.1.2.11.2
Reported vapor pressures and Henry’s law constants of ethylcyclonexane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (1a) \\
\log P &= A - \frac{B}{C + T/K} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (3) \\
\ln P &= A - \frac{B}{C + T/K} \quad (3a) \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

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<tr>
<th>Vapor pressure</th>
<th>Willingham et al. 1945</th>
<th>Stull 1947</th>
<th>Summary of literature data</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
<th>Selected values</th>
<th>From solute fugacity (f) and (x)</th>
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<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
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(Continued)
TABLE 2.1.1.2.11.2 (Continued)

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<tr>
<td>C</td>
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<td></td>
<td></td>
<td>ΔH_V/(kJ mol⁻¹) =</td>
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<td></td>
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<tr>
<td>temp range 51.4–132.7°C</td>
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<td>at 25°C</td>
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<td>pressure range 48–780 mmHg</td>
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<td>at bp</td>
<td>34.31</td>
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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 Cycloheptane

Common Name: Cycloheptane
Synonym: suberane
Chemical Name: cycloheptane
CAS Registry No: 291-64-5
Molecular Formula: C\(_{7}\)H\(_{14}\)
Molecular Weight: 98.186
Melting Point (°C): –12
  –8.46 (Lide 2003)
Boiling Point (°C): 118.5
  118.4 (Lide 2003)
Density (g/cm\(^3\)):
  0.8098 (20°C, Weast 1984)
  0.80656 (measured, Anand et al. 1975)
Molar Volume (cm\(^3\)/mol):
  121.3 (20°C, calculated-density, Stephenson & Malanowski 1987)
  136.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
  4.98, 0.29, 0.45, 1.88 (–138.35, –74.95, –60.75, –8.05°C, Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
  47.6, 48.2 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
  30.0 (shake flask-GC, McAuliffe 1966)
  27.1 (30°C, shake flask-GC, Groves 1988)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
19920* (68.2°C, ebulliometry, measured range 68.2–159°C, Finke et al. 1956)
log (P/mmHg) = 6.85271 – 1330.742/(t°C + 216.246); temp range 68.2–159°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 (P/kPa) = 6.19317 – 1450.17/(T/K – 44.91); temp range 283.048–323.551 K (static method, vapor-liquid equilibria study, Anand et al. 1975)
16312* (63.03°C, comparative ebulliometry, measured range 60–121.7°C, Meyer & Hotz 1976)
log (P/mmHg) = 5.85683 – 1333.780/(t°C + 216.6438); temp range 60–121.7°C (Antoine eq., comparative ebulliometry, Meyer & Hotz 1976)
log (P/atm) = [1– 391.896/(T/K)] \times 10^{0.885524 – 8.19621 \times 10^{-4}\,(T/K) + 7.88065 \times 10^{-7}\,(T/K)^2}; temp range: 284.35–432.17 K (Cox eq., Chao et al. 1983)
2895, 2898 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.97858 – 1331.383/(214.325 + t°C); temp range 60.2–159°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 5.98198 – 1333.899/(216.657 + t°C); temp range 63.03–121.68°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
2895 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.85395 – 1331.57/(216.35 + t°C); temp range: 68–159°C (Antoine eq., Dean 1985, 1992)
2930 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log \( P_{L}/kPa = 5.98143 - 1333.833/(–56.458 + T/K) \); temp range 341–433 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log \( P_{L}/kPa = 6.12682 - 1417.738/(–47.665 + T/K) \); temp range 282–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \( P_{L}/kPa = 5.97596 - 1329.98/(–56.968 + T/K) \); temp range 333–398 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log \( P_{L}/kPa = 7.05325 - 2475.271/(108.392 + T/K) \); temp range 476–604 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

\[
\log (P/\text{mmHg}) = 54.0858 - 3.6109 \times 10^3/(T/K) - 17.331 \cdot \log (T/K) + 7.5292 \times 10^{-3} \cdot (T/K) + 1.7553 \times 10^{-6} \cdot (T/K)^2;
\]

temp range 265–604 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C):

9977 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

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 \( V_M \), 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 \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \) for gas-phase second order rate constants, with \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with \( NO_3 \) radical and \( k_{O_3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference:

\[
k_{OH} = 13.1 \times 10^{-12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at } 298 \text{ K (Atkinson 1985)}
k_{OH} = (7.88 \pm 1.38) \times 10^{-12} \text{cm}^3 \text{mol}^{-1} \text{s}^{-1} \text{ at } 298 \text{ K (flash photolysis-resonance absorption, Jolly et al. 1985)}
k_{OH} = (11.8 - 13.1) \times 10^{-12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at } 298-300 \text{ K (review, Atkinson 1989)}
k_{OH} = 1.25 \times 10^{-11} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1990)}
k_{OH} = 13.0 \times 10^{-12} \text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric \( t_\frac{1}{2} \approx 2.4-24 \text{ h for cycloparaffins, based on the EPA Reactivity Classification of Organics (estimated, Darnall et al. 1976).} \)
TABLE 2.1.1.2.1
Reported vapor pressures of cycloheptane at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\ln P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\ln P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A'[1 - (TB/K)/(T/K)]
\end{align*}
\]

where \( A' = a + bT + cT^2 \)

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<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
<th>t/°C</th>
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\( \Delta H_v = 38.53 \text{ kJ/mol} \) at 25°C

Antoine eq.

\[
\begin{align*}
eq 2 &: P/mmHg \\
A & = 6.85271 \\
B & = 1330.742 \\
C & = 216.246
\end{align*}
\]

Cox eq.

\[
\begin{align*}
eq 5 &: P/atm \\
T_n & = 391.953 \\
a & = 0.839608 \\
-b \times 10^4 & = 6.9133 \\
c \times 10^7 & = 6.4035
\end{align*}
\]

Finke et al. 1956

Anand et al. 1975

Meyer & Hotz 1976

ebulliometric method

static-quartz spiral gauge

comparative ebulliometry

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**FIGURE 2.1.1.2.1** Logarithm of vapor pressure versus reciprocal temperature for cycloheptane.
2.1.1.2.13  Cyclooctane

Common Name: Cyclooctane
Synonym:
Chemical Name: cyclooctane
CAS Registry No: 292-64-8
Molecular Formula: C8H16
Molecular Weight: 112.213
Melting Point (°C):
  14.59  (Lide 2003)
Boiling Point (°C): 151
  149  (Lide 2003)
Density (g/cm³ at 20°C):
  0.8340  (Weast 1984)
Molar Volume (cm³/mol):
  134.4  (20°C, calculated-density, Stephenson & Malanowski 1987)
  154.1  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
  6.32, 0.48, 2.41  (–106.65, –89.35, 14.85°C, Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
  48.89, 51.9  (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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, Mączyński 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/τ + 43.2804·ln τ; τ = T/298.15 K (empirical eq., generator column-GC, Dohányosová et al. 2004)

Vapor Pressure (Pa at 25°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°C, ebulliometry, measured range 96.7–194.4°C, Finke et al. 1956)
log (P/mmHg) = 6.86173 – 1437.682/(t°C + 210.003); temp range 96.7–194.4°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 (P/kPa) = 5.97188 – 1447.45/(T/K – 60.67); temp range 291–323 K (static method, vapor-liquid equilibria VLE study, Anand et al. 1975)
  22454*  (100.133°C, comparative ebulliometry, measured range 100.1–161°C, Meyer & Hotz 1976)
log (P/mmHg) = 5.861786 – 1438.455/(t°C + 210.1844); temp range 100.1–160.9°C (Antoine eq., comparative ebulliometry, Meyer & Hotz 1976)
  767, 740  (extrapolated-Antoine eq., extrapolated, Boublík et al. 1984)
log (P/kPa) = 5.98693 – 1437.751/(210.012 + t°C); temp range 97.6–194.4°C (Antoine eq. from reported expctl. data, Boublík et al. 1984)
log (P/kPa) = 6.06524 – 1492.101/(216.413 + t°C); temp range 100.1–160.9°C (Antoine eq. from reported expctl. data, Boublík et al. 1984)
  740  (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.86187 – 1437.79/(210.02 + t°C); temp range 97–194°C (Antoine eq., Dean 1985, 1992)
  753  (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
log \((P_L/kPa) = 5.98663 - 1437.682/(–63.147 + T/K)\); temp range 369–487 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log \((P_L/kPa) = 5.9899 - 1440.707/(–62.701 + T/K)\); temp range 369–468 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log \((P_L/kPa) = 6.20474 - 1564.985/(–50.842 + T/K)\); temp range 289–369 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry’s Law Constant \((Pa m^3/mol\) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

10485 \((\text{calculated-vapor-liquid equilibrium (VLE data, Yaws et al. 1991)}\)

14526* \((\text{derived from solute fugacity and mole fraction solubility, temp range 273.15–313.15 K, Dohányosová et al. 2004)}\)

Octanol/Water Partition Coefficient, log \(K_{OW}\):

3.28 \((\text{calculated-π substituent constant, Hansch et al. 1968)}\)

3.50 \((\text{calculated-MCI χ, Murray et al. 1975)}\)

3.28 \((\text{Hutchinson et al. 1980; Sangster 1989)}\)

3.28 \((\text{calculated-fragment const., Lyman 1982)}\)

4.45 \((\text{recommended, Sangster 1989)}\)

3.04 \((\text{calculated-molar volume } V_m, \text{ Wang et al. 1992)}\)

4.47 \((\text{calculated-fragment const., Müller & Klein 1992)}\)

3.6117 \((\text{calculated-UNIFAC group contribution, Chen et al. 1993)}\)

Octanol/Air Partition Coefficient, log \(K_{OA}\):

Bioconcentration Factor, log \(BCF\):

Sorption Partition Coefficient, log \(K_{OC}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):

Volatilization:

Photolysis:

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with NO\(_3\) radical and \(k_{O3}\) with O\(_3\) or as indicated, *data at other temperatures see reference:

\(k_{OH} = 14.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (recommended, Atkinson 1997)

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric \(t_{1/2} \sim 2.4–24 \text{ h}\) 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

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<th></th>
<th>Aqueous solubility</th>
<th>Henry’s law constant</th>
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<td>Dohányosová et al. 2004</td>
<td>Dohányosová et al. 2004</td>
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\[
\ln x = A + \frac{B}{\tau} + C \ln \tau
\]  
\[
\tau = \frac{T}{298.15}
\]

**FIGURE 2.1.1.2.13.1** Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for cyclooctane.
Aliphatic and Cyclic Hydrocarbons

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

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \]

\[
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A'\left[1 - \frac{(T_b/K)}{T/K}\right] \quad (5) \text{ where } A' = a + bT + cT^2
\]

Finke et al. 1956
Anand et al. 1975
Meyer & Hotz 1976
Dohányosová et al. 2004

<table>
<thead>
<tr>
<th>t/°C</th>
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Cox equation:

(Continued)
TABLE 2.1.1.2.13.2 (Continued)

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FIGURE 2.1.1.2.13.3 Logarithm of vapor pressure versus reciprocal temperature for cyclooctane.

Cyclooctane: vapor pressure vs. 1/T

- Finke et al. 1956
- Anand et al. 1975
- Meyer & Hotz 1976
- Dohányosová et al. 2004

b.p. = 149 °C
m.p. = 14.59 °C
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: C_{10}H_{18}
Molecular Weight: 138.250

Melting Point (°C):
-42.9  (cis-decalin, Lide 2003)
-30.4  (trans-decalin, Lide 2003)

Boiling Point (°C): 191.7
195.774  (cis-decalin, Camin & Rossini 1955)
187.273  (trans-decalin, Camin & Rossini 1955)
191.7  (Riddick et al. 1986)

Density (g/cm³ at 20°C):
0.8865, 0.8789  (20°C, 25°C, mixed isomers, Riddick et al. 1986)

Molar Volume (cm³/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, ΔHV (kJ/mol):
41.09  (bp, mixed isomers, Riddick et al. 1986)
51.342, 40.999  (cis-decalin, 25°C, bp, Riddick et al. 1986)
49.87, 40.229  (trans-decalin, 25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_fus (kJ/mol):
14.43  (cis-decalin, Chickos et al. 1999)
2.13, 9.49  (trans-decalin, –57.05, 42.95°C, Chickos et al. 1999)

Entropy of Fusion, ΔS_fus (J/mol 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°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
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°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*  (23.3°C, isomer not specified, ebulliometry, measured range 23.3–150.0°C, Gardner & Brewer 1937)
241*  (20°C, cis-decalin, manometry, measured range –29.5 to 194.7°C, Seyer & Mann 1945)
381*  (13°C, trans-decalin, manometry, measured range –30.0 to 235.3°C, Seyer & Mann 1945)
133.3*  (22.5°C, cis-decalin, summary of literature data, temp range 22.5–194.6°C, Stull 1947)
666.6*  (30.6°C, trans-decalin, summary of literature data, temp range –0.80 to 186.7°C, Stull 1947)
5530*  (92.36°C, trans-decalin, ebulliometry, measured range 92.36–187.867°C, Camin & Rossini 1955)
log (P/mmHg) = 6.87529 – 1594.460/(203.392 + t/°C); temp range 99.8–196.4°C (cis-decalin, Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)

log (P/mmHg) = 6.85681 – 1564.683/(206.259 + t/°C); temp range 92.3–187.0°C (trans-decalin, Antoine eq., ebulliometry-manometer measurement, Camin & Rossini 1955)

104*, 164* (cis-decalin, trans-decalin, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.87529 – 1594.81/(203.39 + t/°C), temp range 68–228°C (cis-decalin, Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.86581 – 1564.683/(206.26 + t/°C); temp range 61–219°C (trans-decalin Antoine eq., Dean 1985, 1992)

log (P/atm) = [1– 468.915/(T/K)] × 10^{0.683577 – 0.900942 × 10–4·(T/K) + 2.28255 × 10–7·(T/K)^2}; temp range 295.65–727.59 K (cis-decalin, Cox eq., Chao et al. 1983)


log (P/mmHg) = [–0.2185 × 10515.4/(T/K)] + 7.797540; temp range 22.5–194.6°C (cis-decalin, Antoine eq., Weast 1972–73)

log (P/mmHg) = [–0.2185 × 8749.1/(T/K)] + 6.973042; temp range –0.80 to 186.7°C (trans-decalin, Antoine eq., Weast 1972–73)

log (P/kPa) = 6.96043 – 2358.398/(280.79 + t/°C); temp range –29.5 to 194.7°C (cis-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.98704 – 1568.642/(206.726 + t/°C); temp range 92.36–187.9°C (trans-decalin, Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

log (P/kPa) = 7.69594 – 3126.688/(363.012 + t/°C); temp range –30.0 to 253.3°C (trans-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.00019 – 1594.460/(203.392 + t/°C), temp range not specified (cis-decalin, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 5.98171 – 1564.683/(206.259 + t/°C), temp range not specified (trans-decalin, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 7.69594 – 3126.688/(363.012 + t/°C); temp range 68–228°C (cis-decalin Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.00019 – 1594.460/(203.392 + t/°C), temp range 99.88–196.4°C (cis-decalin, Antoine eq. from reported exptl. data of Camin & Rossini 1955, Boublik et al. 1984)

log (P/kPa) = 5.98171 – 1564.683/(206.259 + t/°C), temp range not specified (trans-decalin, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 7.91576 – 3126.688/(363.012 + t/°C); temp range 68–228°C (cis-decalin Antoine eq., Dean 1985, 1992)

log (P/kPa) = 6.96043 – 2358.398/(280.79 + t/°C); temp range –29.5 to 194.7°C (cis-decalin, Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.98171 – 1564.683/(206.259 + t/°C), temp range not specified (trans-decalin, Antoine eq., Riddick et al. 1986)

log (P/kPa) = 45.6345 – 4.21 × 10^3/(T/K) – 12.881·log (T/K) – 7.8083 × 10^1·(T/K)^2; temp range 230–702 K (cis-decalin, vapor pressure eq., Yaws 1994)

log (P/kPa) = 76.1002 – 5.03 × 10^3/(T/K) – 9.7608 × 10^1·(T/K)^2; temp range 243–687 K (cis-decalin, vapor pressure eq., Yaws 1994)

128* (20.42°C, trans-decalin, differential pressure gauge, measured range –29.31 to 160.7°C, Mokbel et al. 1995)

Henry’s Law Constant (Pa m^3/mol at 25°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°C Ashworth et al. 1988)

ln [H/(atm·m^3/mol)] = 11.85 – 4125/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
Octanol/Water Partition Coefficient, $\log K_{OW}$:
4.79 \hspace{1cm} \text{(calculated-fragment const., Müller & Klein 1992)}

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ as indicated, *data at other temperatures see reference:

$k_{OH} = 1.96 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ of cis-decalin and $2.02 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ of trans-decalin at 299 K (Atkinson 1985)

$k_{OH} = 2.0 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction at 298 K (Atkinson 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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

\[
\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)
\]

\[
\log P = A - B/(C + t/°C) \quad (2) \quad \ln P = A - B/(C + t/°C) \quad (2a)
\]

\[
\log P = A - B/(C + T/K) \quad (3)
\]

\[
\log P = A - B/(T/K) - C\cdot\log (T/K) \quad (4)
\]

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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

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{C + \log (T/K)} \quad (4)
\]

\[
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\ln P = A - \frac{B}{C + T/K} \quad (3a) \\
\ln P = A - \frac{B}{C + \ln (T/K)} \quad (4a)
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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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C \log (T/K)
\end{align*}
\]

(1) \hspace{1cm} (1a) \hspace{1cm} (2) \hspace{1cm} (2a) \hspace{1cm} (3) \hspace{1cm} (4) \hspace{1cm} (4a)

1. Seyer & Mann 1945 – manometry

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2.

Mokbel et al. 1995

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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: C₄H₈; CH₃C(CH₃)CH₂
Molecular Weight: 56.107
Melting Point (°C):
  -140.7  (Lide 2003)
Boiling Point (°C):
  -6.9 (Dreisbach 1959; Lide 2003)
Density (g/cm³ at 20°C):
  0.5942, 0.5879 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
  94.4  (20°C, calculated-density, McAuliffe 1966)
  95.4  (25°C, calculated-density)
  88.8  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₜ (kJ/mol):
  5.92  (Chickos et al. 1999)
Entropy of Fusion, ΔSₘₜ (J/mol K):
  44.72, 41.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  263  (shake flask-GC, of liquid at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at 25°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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<td>log (P/mmHg) = 6.84134 – 923.2/(240.0 + t°C); temp range –68 to 39°C (Antoine eq. for liquid state, Dreisbach 1959)</td>
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log (P/kPa) = 7.64267 – 2336.466/(160.311 + T/K); temp range 371–418 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/mmHg) = 39.2295 – 2.1094 × 10^3/(T/K) – 12.567·log (T/K) + 7.7304 × 10–3·(T/K) – 1.3659 × 10–6·(T/K)^2; temp range 133–418 K (vapor pressure eq., Yaws 1994)

607940 (45.44°C, vapor-liquid equilibrium VLE data, Pasanen et al. 2004)

Henry’s Law Constant (Pa m^3/mol at 25°C):
21600 (calculated-I/Kaw, Cw/Cs, 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 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
20994 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{ow}:
0.64, 1.32 (quoted, calculated-molar volume V_M, Wang et al. 1992)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_0:

Volatilization:

Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{oh} for reaction with OH radical, k_{no3} with NO_3 radical and k_{oj} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:
k_{oh} = 6.2 × 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Hanst et al. 1958)}
k_{oh} = 2.32 × 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 30^\circ\text{C (flow system, Bufalini & Altshuller 1965)}
k_{oh} = 6.46 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (discharge flow system-MS, Morris & Niki 1971)}
k_{oh} = 13.6 × 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{s}^{-1} \text{ at room temp (Japar et al. 1974)}
k_{oh} = 11.7 × 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Huie & Herron 1975)}
k_{oh} = (3.05 ± 0.31) × 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1} \text{ at } 305 ± 2 \text{ K (relative rate method, Winer et al. 1976)}
k_{o3p} = 1.60 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O(P) atoms (Singleton & Cvetanovic 1976; Atkinson & Pitts Jr. 1977; quoted, Gaffney & Levine 1979)}
k_{oh^2} = 5.07 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 297.2 \text{ K, measured range } 297–425 \text{ K (flash photolysis-resonance fluorescence, Atkinson & Pitts 1977)}
k_{oh} = 11.7 × 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 294 ± 2 \text{ K (chemiluminescence, Adeniji et al. 1981)}
k_{oh} = 5.13 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K (relative rate method, Atkinson & Aschmann 1984)}
k_{oh} = (6.46 ± 0.13) × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 ± 2 \text{ K (relative rate method, Ohto 1984)}
k_{oh} = 5.14 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989)}
k_{oh} = 5.14 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{; } k_{o3} = 1.21 × 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (review, Atkinson 1990)}
k_{oh} = 5.14 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{, } k_{o3} = 31.3 × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Sabljic & Güsten 1990)}
k_{o3} = (3.15 – 3.38) × 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1990)}
k_{oh} = 5.14 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{, } k_{o3} = 3.32 × 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{, } k_{o3^*} = 11.3 × 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } k_{o3p} = 1.69 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O(P) atom at } 298 \text{ K (recommended, Atkinson 1997)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) 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 k = 5.14 × 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} with OH radicals in air during summer daylight (Altshuller 1991).
Surface water: $t_{1/2} \approx 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO$_2$ radicals for olefins and $t_{1/2} = 8.0 \text{ d}$ for substituted olefins, based on rate constant $k = 1 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ 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

<table>
<thead>
<tr>
<th>Equation</th>
<th>Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>log $P = A - B/(T/K)$</td>
<td>(1) or (1a)</td>
</tr>
<tr>
<td>log $P = A - B/(C + t/\degree \text{C})$</td>
<td>(2) or (2a)</td>
</tr>
<tr>
<td>log $P = A - B/(T/K) - C\log (T/K)$</td>
<td>(5)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Temperature ($\degree \text{C}$)</th>
<th>Vapor Pressure (Pa)</th>
<th>Temperature ($\degree \text{C}$)</th>
<th>Vapor Pressure (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-56.75</td>
<td>8725</td>
<td>-105.1</td>
<td>133.3</td>
</tr>
<tr>
<td>-25.30</td>
<td>47703</td>
<td>-96.5</td>
<td>666.6</td>
</tr>
<tr>
<td>-20.88</td>
<td>57462</td>
<td>-81.9</td>
<td>1333</td>
</tr>
<tr>
<td>-7.47</td>
<td>99791</td>
<td>-73.4</td>
<td>2666</td>
</tr>
<tr>
<td>-0.67</td>
<td>128789</td>
<td>-63.8</td>
<td>5333</td>
</tr>
<tr>
<td>0.0</td>
<td>131695</td>
<td>-57.7</td>
<td>7999</td>
</tr>
<tr>
<td>0.0</td>
<td>131855</td>
<td>-49.3</td>
<td>13332</td>
</tr>
<tr>
<td>-36.7</td>
<td>26664</td>
<td>-36.7</td>
<td>26664</td>
</tr>
<tr>
<td>0.0</td>
<td>131855</td>
<td>-49.3</td>
<td>13332</td>
</tr>
<tr>
<td>0.0</td>
<td>131855</td>
<td>-49.3</td>
<td>13332</td>
</tr>
</tbody>
</table>

Lamb & Roper 1940
Stull 1947
Zwolinski & Wilhoit 1971

Static method-manometer
Summary of literature data
Selected values

bp/°C: -7.12
A: 9.77465
B: 1503.866
C: 0.0046649

2-Methylpropene: vapor pressure vs. 1/T

Logarithm of vapor pressure versus reciprocal temperature for 2-methylpropene.

FIGURE 2.1.2.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methylpropene.
Common Name: 1-Butene
Synonym: butylene
Chemical Name: 1-butene
CAS Registry No: 106-98-9
Molecular Formula: \( \text{C}_4\text{H}_8; \text{CH}_3\text{CH}_2\text{CHCH}_2 \)
Molecular Weight: 56.107
Melting Point (°C):
-185.34 (Lide 2003)
Boiling Point (°C):
-6.26 (Dreisbach 1959; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
0.5951, 0.5888 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
94.3 (20°C, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)
95.3 (25°C, calculated-density)
88.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
3.85 (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
43.84, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
222 (shake flask-GC, liquid at 1 atmospheric pressure, McAuliffe 1966)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
128536* (0°C, static method-manometer, measured range –56.75 to 0°C, Lamb & Roper 1940)
log (P/mmHg) = –1330.977/(T/K) – 0.0017607·(T/K) + 8.33816; temp range 195–274 K (static method, Lamb & Roper 1940)
361100* (Antoine eq. regression, temp range –104.8 to –6.3°C, Stull 1947)
296000 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.84290 – 926.1/(240.0 + t°C); temp range –67 to 40°C (Antoine eq. for liquid state, Dreisbach 1959)
297309* (derived from compiled data, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.84290 – 926.10/(240.00 + t°C); temp range –81.5 to 12.6°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 5996.7/(T/K)] + 7.826754; temp range –104.8 to –6.3°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = 6.531 – 810.261/(228.066 + t°C) (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/mmHg) = 6.79290 – 908.80/(238.54 + t°C); temp range –82 to 13°C (Antoine eq., Dean 1985, 1992)
297020, 295800 (interpolated-Antoine eq.-III, V, Stephenson & Malanowski 1987)
log (P/\text{Pa}) = 5.9678 – 926.1/(-33.15 + T/K); temp range 200–274 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/\text{Pa}) = 8.1706 – 1601.52/(7.059 + T/K); temp range 126–192 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/\text{Pa}) = 6.05416 – 970.771/(-27.089 + T/K); temp range 267–345 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/\text{Pa}) = 6.77294 – 1482/801/(48.073 + T/K); temp range 342–411 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
log (P/\text{Pa}) = 6.27411 – 1097.171/(-9.657 + T/K); temp range 267–411 K (Antoine eq.-V, Stephenson & Malanowski 1987)
\[
\log (P/\text{mmHg}) = 27.3116 - 1.9235 \times 10^9/(T/K) - 70.2064 \log (T/K) + 3.6481 \times 10^{-6}(T/K)^2;
\]

temp range 88–420 K (vapor pressure eq., Yaws 1994)

596140 (50.12°C, vapor-liquid equilibrium VLE data, Pasanen et al., 2004)

Henry’s Law Constant (Pa m³/mol at 25°C):

25610 (calculated-P/C, Mackay & Shiu 1981)

25370 (calculated-1/K_{AW}, C_{AW}/C_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, \( \log K_{OW} \):

2.40; 2.17, 2.26, 2.43 (quoted; calculated-f const., Rekker 1977)

1.59, 1.32 (quoted, calculated-molar volume \( V_M \), Wang et al. 1992)

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with \( OH \) radical, \( k_{NO_3} \) with \( NO_3 \) radical and \( k_{O(3P)} \) with \( O(3P) \) atom, or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\( k_{OH} = 1.03 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 30°C (flow system, Bufalini & Altshuller 1965)

\( k_{OH} = 4.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (discharge flow system-MS, Morris & Niki 1971)

\( k_{O(3P)} = 4.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) for the reaction with \( O(3P) \) atom (Singleton & Cvetanovic 1976; Atkinson & Pitts Jr. 1977; quoted, Gaffney & Levine 1979)

\( k_{OH} = 3.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 297.2 K, measured range 297–425 K (flash photolysis-resonance fluorescence, Atkinson & Pitts, Jr. 1977)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 295 K (relative rate method, Atkinson & Aschmann 1984)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1989)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Atkinson 1990)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Sabljic & Güsten 1990)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with an estimated lifetime of 5.5 h during summer daylight hours (Altshuller 1991)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with an estimated lifetime of 5.5 h during summer daylight hours (Altshuller 1991)

\( k_{OH} = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with an estimated lifetime of 5.5 h during summer daylight hours (Altshuller 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) 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 \( k = 3.14 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with \( OH \) radicals during summer daylight in the gas phase (Altshuller 1991).
Surface water: $t_{1/2} = 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for reaction with OH and RO$_2$ radicals of olefins in aquatic system, and $t_{1/2} = 7.3 \text{ d}$, based on oxidation reaction rate constant $k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ with singlet 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\log (T/K) \quad (4) \\
\log P &= A - B/(T/K) - C(T/K) \quad (5)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Lamb &amp; Roper 1940</th>
<th>Stull 1947</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>static method-manometer</strong></td>
<td><strong>summary of literature data</strong></td>
<td><strong>selected values</strong></td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$P/Pa$</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>(-56.75)</td>
<td>8549</td>
<td>(-104.8)</td>
</tr>
<tr>
<td>(-25.3)</td>
<td>45423</td>
<td>(-89.4)</td>
</tr>
<tr>
<td>(-22.91)</td>
<td>50436</td>
<td>(-81.6)</td>
</tr>
<tr>
<td>(-10.60)</td>
<td>85513</td>
<td>(-73.0)</td>
</tr>
<tr>
<td>(-7.47)</td>
<td>96992</td>
<td>(-63.4)</td>
</tr>
<tr>
<td>(-0.67)</td>
<td>125549</td>
<td>(-57.2)</td>
</tr>
<tr>
<td>0.0</td>
<td>128536</td>
<td>(-48.9)</td>
</tr>
<tr>
<td>(\text{b.p.}/°C)</td>
<td>(-6.30)</td>
<td>(-36.2)</td>
</tr>
<tr>
<td>(\text{eq. 5})</td>
<td>(\text{P/mmHg})</td>
<td>(-6.3)</td>
</tr>
<tr>
<td>A</td>
<td>6.33816</td>
<td>(-6.3)</td>
</tr>
<tr>
<td>B</td>
<td>1330.977</td>
<td>(-130)</td>
</tr>
<tr>
<td>C</td>
<td>0.0017607</td>
<td>(-21.62)</td>
</tr>
<tr>
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</tbody>
</table>

\[\Delta H_v/(kJ \text{ mol}^{-1}) = \]

\[\begin{align*}
\text{b.p.} &= -6.26 °C \\
\text{at bp} &= 21.92
\end{align*}\]

**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: C₅H₁₀, CH₃CH₂C(CH₃)CH₂
Molecular Weight: 70.133
Melting Point (°C):
   -137.53 (Lide 2003)
Boiling Point (°C):
   31.2 (Lide 2003)
Density (g/cm³ at 20°C):
   0.6504, 0.6451 (20°C, 25°C, at saturation pressure, Dreisbach 1959; Dean 1985)
Molar Volume (cm³/mol):
   107.8, 108.7 (20°C, 25°C, calculated-density)
   111.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₚₒₛ (kJ/mol):
   7.91 (Chickos et al. 1999)
Entropy of Fusion, ΔSₚₒₛ (J/mol K):
   58.34, 48.9 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
   215* (20°C, shake flask-GC, measured range 20–60°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 Vₘₐₙ, Wang et al. 1992)
   128, 198 (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
Vapor Pressure (Pa at 25°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°C, Stull 1947)
   70242* (20.996°C, ebulliometry, measured range 1.155–62.675°C, Scott et al. 1949)
   log (P/mmHg) = 6.87314 – 1053.780/(232.768 + t°C); temp range 1.155 to 62.675°C (Antoine eq., ebulliometry, Scott et al. 1949)
   81320 (calculated from determined data, Dreisbach 1959)
   log (P/mmHg) = 6.87314 – 1053.8/(233.0 + t°C); temp range –38 to 75°C (Antoine eq. for liquid state, Dreisbach 1959)
   81327*, 81330 (derived from compiled data, interpolated-Antoine eq., temp range –53.4 to 52.24°C Zwolinski & Wilhoit 1971)
   log (P/mmHg) = 6.87314 – 1053.780/(232.788 + t°C); temp range –53.4 to 52.24°C (Antoine eq., Zwolinski & Wilhoit 1971)
   log (P/mmHg) = [–0.2185 × 6474.6/(T/K)] + 7.751419; temp range –89.1 to 20.2°C (Antoine eq., Weast 1972–73)
   82830 (interpolated-Antoine eq., Boublík et al. 1984)
   log (P/Pa) = 5.98334 – 1046.771/(232.181 + t°C) temp range 1.115–63.68°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
   99500 (interpolated-Antoine eq., temp range –53 to 52°C, Dean 1985, 1992)
   log (P/mmHg) = 6.84637 – 1039.69/(236.65 + t°C); temp range –53 to 52°C (Antoine eq., Dean 1985, 1992)
   81360 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
Aliphatic and Cyclic Hydrocarbons

\[
\log \left( \frac{P}{kPa} \right) = 5.99292 - 1050.937/(–40.727 + T/K); \text{ temp range 240–336 K (Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log \left( \frac{P}{mmHg} \right) = 30.2418 - 2.2723 \times 10^{3}/(T/K) - 8.1482 \times \log (T/K) + 5.2331 \times 10^{-11} \times (T/K) + 3.6802 \times 10^{-6} \times (T/K)^{2}; \text{ temp range 136–465 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°C):

43080 (calculated-MCI \( \chi \), Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, log \( K_{ow} \):

2.07 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
1.89 (calculated-molar volume \( V_{M} \), Wang et al. 1992)

Octanol/Air Partition Coefficient, log \( K_{oa} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_3 radical and \( k_{O3} \) with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[
k_{OH} = 9.01 \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (discharge flow system-MS, Morris & Niki 1971)}
\]

\[
k_{OH} = (6.37 \pm 0.16) \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K ± 2 K (relative rate method, Ohta 1984)}
\]

\[
k_{OH} = 9.01 \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ to } 6.07 \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (review, Atkinson 1985)}
\]

\[
k_{OH} = (60.7 - 90.1) \times 10^{-12} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (review, Atkinson 1989)}
\]

\[
k_{OH} = 6.10 \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ with an estimated atmospheric lifetime of 2.3 h during summer daylight hours (Altshuller 1991)}
\]

\[
k_{OH} = 6.1 \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1}, \text{ and } k_{O3} = 16.0 \times 10^{-18} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1997)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_{u} \)) and Elimination (\( k_{e} \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric lifetime \( \tau \sim 2.3 \text{ h}, \) based on the photooxidation rate constant \( k = 6.10 \times 10^{-11} \text{ cm}^{3} \text{ molecule}^{-1} \text{ s}^{-1} \) with hydroxyl radical in air during summer daylight (Altshuller 1991).

Surface water: \( t_{1/2} = 320 \text{ h and } 9 \times 10^{4} \text{ d for reaction with OH and RO_{2} radicals for olefins in aquatic system, and } t_{1/2} = 7.3 \text{ d, based on oxidation reaction rate constant of } 3 \times 10^{7} \text{ M}^{-1} \text{ s}^{-1} \) 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

<table>
<thead>
<tr>
<th>Pavlova et al. 1966</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Shake flask-GC</strong></td>
</tr>
<tr>
<td>( t/°C ) &amp; ( S/g·m^{–3} )</td>
</tr>
<tr>
<td>20 &amp; 215</td>
</tr>
<tr>
<td>40 &amp; 326</td>
</tr>
<tr>
<td>50 &amp; 250</td>
</tr>
<tr>
<td>60 &amp; 267</td>
</tr>
</tbody>
</table>

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FIGURE 2.1.2.1.3.1 Logarithm of mole fraction solubility (ln 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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\end{align*}
\]

Stull 1947
Scott et al. 1949
Zwolinski & Wilhoit 1971

<table>
<thead>
<tr>
<th>summary of literature data</th>
<th>ebulliometry</th>
<th>selected values</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>-89.1</td>
<td>133.3</td>
<td>1.155</td>
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<tr>
<td>-72.8</td>
<td>666.6</td>
<td>6.054</td>
</tr>
<tr>
<td>-64.3</td>
<td>1333</td>
<td>10.993</td>
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<td>-54.8</td>
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<td>-44.1</td>
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<td>-37.3</td>
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<tr>
<td>-28.0</td>
<td>13332</td>
<td>31.162</td>
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<tr>
<td>-13.8</td>
<td>26664</td>
<td>36.308</td>
</tr>
<tr>
<td>2.5</td>
<td>53329</td>
<td>41.500</td>
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<tr>
<td>20.2</td>
<td>101325</td>
<td>46.728</td>
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<tr>
<td>mp/°C</td>
<td>-135</td>
<td>52.005</td>
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<tr>
<td>bp/°C</td>
<td>31.16</td>
<td>57.320</td>
</tr>
<tr>
<td>Antoine eq.</td>
<td>eq. 2</td>
<td>62.675</td>
</tr>
<tr>
<td>P/mmHg</td>
<td>29.620</td>
<td>28.623</td>
</tr>
</tbody>
</table>
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: C₅H₁₀, (CH₃)₂CHCH=CH₂
Molecular Weight: 70.133
Melting Point (°C):
  –168.43 (Lide 2003)
Boiling Point (°C):
  20.1 (Lide 2003)
Density (g/cm³ at 20°C):
  0.6272, 0.6219 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
  111.8 (20°C, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)
  111.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
  5.36 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
  51.19, 41.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F:
  1.0
Water Solubility (g/m³ or mg/L at 25°C):
  130 (shake flask-GC, McAuliffe 1966)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
  101325 (20.2°C, summary of literature data, temp range –89.1 to 20.2°C, Stull 1947)
  120790* (25.128°C, ebulliometry, measured range 0.218–51.139°C, Scott & Waddington 1950)
log (P/mmHg) = 6.82618 – 1013.474/(236.816 + t/°C); temp range 0.219–51.139°C (Antoine eq., ebulliometric method, Scott & Waddington 1950)
  120260 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.82618 – 1013.474/(237.0 + t/°C); temp range –47 to 60°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°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.82618 – 1013.474/(236.816 + t/°C); temp range –62.9 to 60°C (Antoine eq. for liquid state, Zwolinski & Wilhoit 1971)
  120180 (interpolated-Antoine eq., temp range –63 to 41°C, Dean 1985, 1992)
log (P/mmHg) = 6.82455 – 1012.37/(236.65 + t/°C); temp range –63 to 41°C (Antoine eq., Dean 1985, 1992)
  120300 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/P₀) = 5.94656 – 1010.866/(–36.694 + T/K); temp range 237–324 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 31.1486 – 2.1764 × 10⁻³/(T/K) – 8.5146·log (T/K) + 5.9672 × 10⁻¹(T/K) + 4.7555 × 10⁻⁶(T/K)²; temp range 105–450 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
  54230 (calculated-1/K_{AW}, C_W/C_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 χ, Nirmalakhandan & Speece 1988)
Octanol/Water Partition Coefficient, log $K_{OW}$:

- 2.05 (calculated-molar volume $V_M$, Wang et al. 1992)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

**Volatilization:**

**Photolysis:**

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

- $k_{OH} = (3.10 \pm 0.31) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 299.2 K, measured range 299–433 K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)
- $k_{O(3P)} = 4.30 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction with O(3P) atom (Singleton & Cvetanovic 1976; quoted, Gaffney & Levine 1979)
- $k_{OH} = 3.18 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1984)
- $k_{OH} = 9.01 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $6.07 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1985)
- $k_{OH} = 3.18 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)
- $k_{NO3} = 9.8 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson 1991)
- $k_{OH} = 3.18 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{O3} = 11.0 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{O(3P)} = 4.15 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with O(3P) atom at 298 K (recommended, Atkinson 1997)

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} = 320$ h and $9 \times 10^4$ d for reaction with OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 7.3$ d, based on oxidation reaction rate constant $k = 3 \times 10^3$ M$^{-1}$ 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

\[
\log P = A - \frac{B}{(T/K)} \quad (1) \\
\ln P = A - \frac{B}{(T/K)} \quad (1a) \\
\log P = A - \frac{B}{(C + T/K)} \quad (2) \\
\ln P = A - \frac{B}{(C + T/K)} \quad (2a) \\
\log P = A - \frac{B}{(C + t/°C)} \quad (3) \\
\ln P = A - \frac{B}{(C + t/°C)} \quad (3a) \\
\log P = A - \frac{B}{(T/K)} - C \cdot \log (T/K) \quad (4)
\]

**Scott & Waddington 1950**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.210</td>
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<td>20.06</td>
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</tr>
<tr>
<td>5.112</td>
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<td>Antoine eq.</td>
<td>600</td>
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<td>eq. 2</td>
<td>70109</td>
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<tr>
<td>15.033</td>
<td>84158</td>
<td>A</td>
<td>84158</td>
</tr>
<tr>
<td>20.061</td>
<td>101325</td>
<td>B</td>
<td>101325</td>
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<tr>
<td>25.128</td>
<td>120790</td>
<td>C</td>
<td>120790</td>
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<tr>
<td>51.139</td>
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<td></td>
</tr>
</tbody>
</table>

**Zwolinski & Wilhoit 1971**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
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<tr>
<td>62.9</td>
<td>1333</td>
<td>17.757</td>
<td>93326</td>
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<tr>
<td>53.4</td>
<td>2666</td>
<td>18.541</td>
<td>95992</td>
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<tr>
<td>47.3</td>
<td>4000</td>
<td>19.309</td>
<td>98659</td>
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<td>42.6</td>
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<td>101325</td>
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<td>7999</td>
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<td>30.96</td>
<td>10666</td>
<td>eq. 2</td>
<td>P/mmHg</td>
</tr>
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<td>26.82</td>
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<td>A</td>
<td>6.82618</td>
</tr>
<tr>
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<td>19998</td>
<td>B</td>
<td>1013474</td>
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<tr>
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<td>26664</td>
<td>C</td>
<td>236366</td>
</tr>
<tr>
<td>7.95</td>
<td>33331</td>
<td>b.p./°C</td>
<td>20.061</td>
</tr>
<tr>
<td>-3.783</td>
<td>39997</td>
<td>ΔHᵥ/Δ (kJ mol⁻¹) = 3.109 53329 at 25°C 23.85</td>
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</tr>
<tr>
<td>8.743</td>
<td>66661</td>
<td>at b.p. 24.06</td>
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</table>

**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: 2-methyl-2-butene
Chemical Name: 2-methyl-2-butene
CAS Registry No: 513-35-9
Molecular Formula: C5H10, CH3CH=C(CH3)CH3
Molecular Weight: 70.133
Melting Point (°C):
–133.72 (Lide 2003)
Boiling Point (°C):
38.56 (Lide 2003)
Density (g/cm³ at 20°C):
0.6623, 0.6570 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
105.9, 106.8 (20°C, 25°C, calculated-density)
111.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hfus (kJ/mol):
7.60 (Chickos et al. 1999)
Entropy of Fusion, ∆Sfus (J/mol K):
54.47, 59.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):
215* (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
47876* (18.07°C, static method, measured range –78.85 to 18.07°C, Lamb & Roper 1940)
\[ \log (P/\text{mmHg}) = 9.86840 - 1773.506/(T/\text{K}) + 0.0035747 \log (T/\text{K}); \text{ temp range } -78.85 \text{ to } 18.07 \text{°C} \] (static method, Lamb & Roper 1940)
53329* (21.6, summary of literature data, temp range –75.4 to 38.5°C, Stull 1947)
57798* (ebulliometry, measured range 3.042 to 70.59°C, Scott et al. 1949)
\[ \log (P/\text{mmHg}) = 6.91562 - 1095.088/(232.842 + t/°C); \text{ temp range } 3.04 \text{ to } 70.59 \text{°C} \] (Antoine eq., ebulliometry, Scott et al. 1949)
62140 (calculated-Antoine eq., Dreisbach 1959)
\[ \log (P/\text{mmHg}) = 6.91562 - 1095.088/(233.0 + t/°C); \text{ temp range } -31 \text{ to } 85 \text{°C} \] (Antoine eq. for liquid state, Dreisbach 1959)
62142*, 62140 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 6.91562 - 1095.088/(232.842 + t/°C); \text{ temp range } -47.7 \text{ to } 60.0 \text{°C} \] (Antoine eq., Zwolinski & Wilhoit 1971)
62890, 62140 (calculated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{kPa}) = 6.15017 - 1146.28/(238.416 + t/°C); \text{ temp range } -78.85 \text{ to } 18.07 \text{°C} \] (Antoine eq. from reported exptl. data, Boublik et al. 1984)
\[ \log (P/\text{kPa}) = 6.04808 - 1099.054/(233.314 + t/°C); \text{ temp range } 3.04 \text{ to } 70.59 \text{°C} \] (Antoine eq. from reported exptl. data, Boublik et al. 1984)
62240 (interpolated-Antoine eq., Dean 1985, 1992)
\[ \log (P/\text{mmHg}) = 6.96659 - 1124.33/(236.63 + t/°C); \text{ temp range } -48 \text{ to } 60 \text{°C} \] (Antoine eq., Dean 1985, 1992)
62170 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
\[
\log (P_{\text{atm}}/\text{kPa}) = 6.04475 - 1097.501/(T/\text{K}) + 9.8429\log (T/\text{K}) + 4.7156 \times 10^{-6}(T/\text{K})^2;
\]

temp range 193–471 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
\[
24650 \quad \text{(calculated-P/C from selected data)}
\]

Octanol/Water Partition Coefficient, \(\log K_{\text{OW}}\):

Octanol/Air Partition Coefficient, \(\log K_{\text{OA}}\):

Bioconcentration Factor, \(\log BCF\):

Sorption Partition Coefficient, \(\log K_{\text{OC}}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_\text{1/2}\):

**Volutilization:**

**Photolysis:**

**Oxidation:** rate constant \(k\); for gas-phase second-order rate constants, \(k_{\text{OH}}\) for reaction with OH radical, \(k_{\text{NO3}}\) with NO_3 radical and \(k_{\text{O(3P)}}\) with O_3 atom as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\(k_{\text{OH}} = 7.47 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 30°C (flow system, Bufalini & Altshuller 1965)

\(k_{\text{OH}} = 11.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (discharge flow system-MS, Morris & Niki 1971)

\(k_{\text{O(3P)}} = 5.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with the rate constant for reaction with O(P) (Herron & Huie 1973; Furuyama et al. 1974; Atkinson & Pitts Jr. 1978; quoted, Gaffney & Levine 1979)

\(k_{\text{OH}} = 4.93 \times 10^{-16} \text{ cm}^3 \text{ molelcule}^{-1} \text{ s}^{-1} \) at 299 K (Japar et al. 1974)

\(k_{\text{OH}} = 4.8 \times 10^6 \text{ L molecule}^{-1} \text{ s}^{-1}\) with atmospheric \(t_{\text{OH}} < 0.24 \text{ h}\) (Darnall et al. 1976, Lloyd et al. 1976)

\(k_{\text{OH}} = 8.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)

\(k_{\text{OH}} = 8.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\); \(k_{\text{O(3P)}} = 5.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at room temp. (LFE correlation, Gaffney & Levine 1979)

\(k_{\text{OH}} = (87.1 \pm 2.6) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 297 ± 2 K (relative rate method, Ohta 1984)

\(k_{\text{NO3}} = (5.5 \pm 1.2) \times 10^{-12} \text{ cm}^3 \text{ molelcule}^{-1} \text{ s}^{-1} \) at 295 K (relative rate method, Atkinson et al. 1984a)

\(k_{\text{NO3}} = 4.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with calculated lifetimes \(\tau = 55 \text{ min}\) and 17 min in clean and moderately polluted atmosphere respectively, \(k_{\text{OH}} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with calculated lifetimes \(\tau = 3.2 \text{ h}\) and 1.6 h in clean and moderately polluted atmosphere, respectively; \(k_{\text{NO3}} = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with calculated lifetimes \(\tau = 13 \text{ min}\) and 1.3 min in clean and moderately polluted atmosphere, respectively (Atkinson et al. 1984a)

\(k_{\text{O(3P)}} < 0.5 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 295 K (Atkinson et al. 1984b)

\(k_{\text{O(3P)}} = 4.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\); \(k_{\text{OH}} = 8.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\); \(k_{\text{NO3}} = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\); and \(k_{\text{O(3P)}} = 47.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with O(P) atom at room temp. (Atkinson et al. 1984b)

\(k_{\text{OH}} = 6.86 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 295 ± 1 K (relative rate method, Atkinson & Aschmann 1984)

\(k_{\text{OH}} = (6.79–7.97) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296–299 K (Atkinson & Carter 1984)

\(k_{\text{OH}} = 4.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with a loss rate of 25 d^{-1}; \(k_{\text{OH}} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with a loss rate of 25 d^{-1} (Atkinson & Carter 1984)

\(k_{\text{OH}} = 7.7 \times 10^{-11} \text{ to } 1.19 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) between 297.7–299.5 K (Atkinson 1985)

\(k_{\text{OH}} = 4.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with a loss rate of 25 d^{-1}; \(k_{\text{OH}} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with a loss rate of 3.8 d^{-1}, and \(k_{\text{NO3}} = 9.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) with a loss rate of 205 d^{-1} at room temp (Atkinson 1985)

\(k_{\text{NO3}} = (9.33 \pm 1.18) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 296 ± 2 K (relative rate method, Atkinson 1988)

\(k_{\text{OH}} = 8.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 298 K (recommended, Atkinson 1989)

\(k_{\text{OH}} = 6.89 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\); \(k_{\text{NO3}} = 4.23 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 198 K (Atkinson 1990)

\(k_{\text{OH}} = 8.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\); \(k_{\text{NO3}} = 9.33 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) at 289 K (Sabljic & Güsten 1990)
Aliphatic and Cyclic Hydrocarbons

\[ k_{\text{NO}_3} = 9.37 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1991)} \]

\[ k_{\text{OH}^*} = 8.69 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{\text{NO}_3} = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad k_{\text{O}_3^*} = 4.03 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \quad \text{and } k_{\text{O}(3\text{P})} = 5.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O}(3\text{P}) \text{ atom at } 298 \text{ K (recommended, Atkinson 1997))} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric \( t_{1/2} < 0.24 \text{ h} \), based on the photooxidation rate constant \( k = 4.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \) with hydroxyl radical in air (Darnall et al. 1976; Lloyd et al. 1976); atmospheric lifetimes, \( \tau(\text{calc}) = 0.95 \text{ h} \) for the reaction with \( \text{O}_3 \), \( \tau = 3.2 \text{ h} \) with \( \text{OH} \) radical and \( \tau = 0.12 \text{ h} \) with \( \text{NO}_3 \) radical, based on the rate constants and environmental concentrations of \( \text{OH}, \text{O}_3 \), and \( \text{NO}_3 \) in the gas phase (Atkinson & Carter 1984);

calculated lifetimes: \( \tau = 55 \text{ min} \) due to reaction with \( \text{O}_3 \) in 24-h period, \( \tau = 3.2 \text{ h} \) with \( \text{OH} \) radical during daytime, and \( \tau = 13 \text{ min} \) for \( \text{NO}_3 \) radical during nighttime for “clean” atmosphere; \( \tau = 17 \text{ min} \) for reaction with \( \text{O}_3 \) in 24-h period, \( \tau = 1.6 \text{ h} \) with \( \text{OH} \) radical during daytime, and \( \tau = 1.3 \text{ min} \) with \( \text{NO}_3 \) radical during nighttime in “moderately” polluted atmosphere (Atkinson et al. 1984a);

atmospheric lifetimes \( \tau(\text{calc}) = 6.38 \text{ h} \) for the reaction with \( \text{OH} \) radical, \( \tau(\text{calc}) = 0.92 \text{ h} \) with \( \text{O}_3 \) and \( \tau(\text{calc}) = 0.12 \text{ h} \) with \( \text{NO}_3 \) radical in the gas phase (Atkinson 1985).

Surface water: \( t_{1/2} \sim 320 \text{ h} \) and \( 9 \times 10^4 \text{ d} \) for reaction with \( \text{OH} \) and \( \text{RO}_2 \) radicals respectively in aquatic system, and \( t_{1/2} = 8.0 \text{ d} \), based on rate constant of \( 10^6 \text{ M}^{-1} \text{ s}^{-1} \) for the reaction with singlet oxygen in aquatic system (Mill & Mabey 1985).

<table>
<thead>
<tr>
<th>Table 2.1.2.1.5.1</th>
<th>Reported aqueous solubilities of 2-methyl-2-butene at various temperatures</th>
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<tr>
<td>Pavlova et al. 1966</td>
<td>Góral et al. 2004</td>
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FIGURE 2.1.2.1.5.1 Logarithm of mole fraction solubility (ln 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

\[
\log P = A - \frac{B}{T/K} \quad (1) \quad \ln P = A - \frac{B}{T/K} \quad (1a)
\]
\[
\log P = A - \frac{B}{C + t/°C} \quad (2) \quad \ln P = A - \frac{B}{C + t/°C} \quad (2a)
\]
\[
\log P = A - \frac{B}{C + T/K} \quad (3)
\]
\[
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]
\[
\log P = A - \frac{B}{T/K} - C \cdot \left(\frac{T}{K}\right) \quad (5)
\]

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<tr>
<th>Lamb &amp; Roper 1940</th>
<th>Stull 1947</th>
<th>Scott et al. 1949</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
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<td>Ebulliometry</td>
<td>Selected values</td>
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</table>

bp/°C 38.43 31.834 79993
eq. 5 P/mmHg 38.43 36.187 93326
A 9.68640 36.187 95992
B 1773.506 37.991 98659
C 0.0035747 38.568 101325
TABLE 2.1.2.1.5.2 (Continued)

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<th>Stull 1947</th>
<th>Scott et al. 1949</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
</tr>
</thead>
<tbody>
<tr>
<td>Static method-manometer</td>
<td>Summary of literature data</td>
<td>Ebulliometry</td>
<td>Selected values</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
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<td>P/mmHg</td>
</tr>
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<td>27.06</td>
<td>at bp</td>
<td>26.30</td>
</tr>
</tbody>
</table>

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, α-n-amylene, propylene
Chemical Name: 1-pentene
CAS Registry No: 109-67-1
Molecular Formula: C₅H₁₀
Molecular Weight: 70.133

Melting Point (°C):
  −165.12 (Lide 2003)

Boiling Point (°C):
  29.96 (Lide 2003)

Density (g/cm³):
  0.6405, 0.63533 (20°C, 25°C, Forziati et al. 1950, Dreisbach 1959)
  0.6353 (20°C, Riddick et al. 1986)

Molar Volume (cm³/mol):
  109.5 (20°C, calculated-density, Stephenson & Malanowski 1987)
  111.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆HV (kJ/mol):

Enthalpy of Fusion, ∆Hfus (kJ/mol):
  5.998 (Riddick et al. 1986)
  5.81 (Chickos et al. 1999)

Entropy of Fusion, ∆Sfus (J/mol K):
  53.82, 54.4 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
  148 (shake flask-GC, McAuliffe 1966)
  191 (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°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°C, Stull 1947)
70834 (20°C, static method, measured range 0–200°C, Day et al. 1948)
log (P/mmHg) = 7.40607 − 1372.194/(T/K); temp range 0–30°C (static method, Day et al. 1948)
log (P/mmHg) = 7.31561 − 1342.407/(T/K); temp range 40–95°C (static method, Day et al. 1948)
84508* (ebulliometry, measured range −0.159 to 61.64°C, Scott et al. 1949)
log (P/mmHg) = 6.85487 − 1049.00/(233.994 + t/°C); temp range −63 to 41°C (Antoine eq., ebulliometry, Scott et al. 1949)
83750* (24.6°C, ebulliometry-manometer, measured range 12.8–30.7°C, Forziati et al. 1950)
log (P/mmHg) = 6.78568 − 1014.293/(229.783 + t/°C); temp range 12.8–30.7°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
86500 (calculated from determined data, Dreisbach 1959)
log (P/mmHg) = 6.84650 − 1044.9/(233.40 + t/°C); temp range −39 to 73°C (Antoine eq. for liquid state, Dreisbach 1959)
85000* (interpolated-Antoine eq., temp range −63 to 41°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.84650 − 1044.895/(233.516 + t/°C); temp range −63 to 41°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [−0.2185 × 6931.2/(T/K)] + 7.914969; temp range −80.4 to 30.1°C (Antoine eq., Weast 1972–73)
85020 (interpolated-Antoine eq., Boublík et al. 1984)

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log (P/kPa) = 5.9716 – 1045.212/(233.598 + t/°C); temp range 12.84–30.7°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublík et al. 1984)
85200 (interpolated-Antoine eq., temp range –55 to 51°C, Dean 1985, 1992)
log (P/mmHg) = 6.84424 – 1044.015/(233.50 + t/°C); temp range –55 to 51°C (Antoine eq., Dean 1985, 1992)
85100 (literature average, Riddick et al. 1986)
log (P/kPa) = 5.96914 – 1044.01/(233.49 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)
85040 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 36.2741 – 2.4452 × 103/(T/K) – 10.405·log (T/K) – 7.4629 × 10–11·(T/K)2; temp range 110–465 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol at 25°C):
40330 (calculated-P/C, Mackay & Shiu 1975; selected, Mills et al. 1982)
41140 (calculated as 1/KAW, Cw/Ca, 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 χ, 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 K ow:
2.20 (calculated-π substituent constant, Hansch et al. 1968)
2.69 (calculated-f const., Yalkowsky & Morozowich 1980)
2.20 (calculated-MCI χ, 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 KOA at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
2.0* (20.29°C, from GC determined γ∞ in octanol, measured range 20.29–50.2°C, Gruber et al. 1997)
1.93 (calculated-measured γ∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:
Volatilization:
Photolysis:
Oxidation: rate constant k for gas-phase second order rate constants, kOH for reaction with OH radical, kNO3 with NO3 radical and kO3 with O3 or as indicated, *data at other temperatures see reference:
kOH = 4.25 × 10–11 cm3 molecule–1 s–1 at 298 K (discharge flow system-MS, Morris & Niki 1971)
kO3 = 1.07 × 10–17 cm3 molecule–1 s–1 (Japar et al. 1974)
kO3 = 5.3 × 10–18 cm3 molecule–1 s–1, 7.4 × 10–18 cm3 molecule–1 s–1, and 1.07 × 10–17 cm3 molecule–1 s–1 (review, Atkinson & Carter 1984)
kOH = 3.13 × 10–11 cm3 molecule–1 s–1 at 295 K (relative rate method, Atkinson & Aschmann 1984)
kOH = 3.14 × 10–11 cm3 molecule–1 s–1 at 298 K (recommended, Atkinson 1989)
kOH = 3.14 × 10–11 cm3 molecule–1 s–1, kO3 = 1.10 × 10–17 cm3 molecule–1 s–1 at 298 K (Atkinson 1990)
kO3 = 1.00 × 10–17 cm3 molecule–1 s–1 at 298 K (recommended, Atkinson 1994)
kOH = 3.14 × 10–11 cm3 molecule–1 s–1, kO3* = 10.0 × 10–18 cm3 molecule–1 s–1, and kO(3P) = 4.65 × 10–12 cm3 molecule–1 s–1 for reaction with O(3P) atom at 298 K (recommended, Atkinson 1997)
Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Surface water: \( t_{1/2} \approx 320 \) h and \( 9 \times 10^4 \) d for olefins in aquatic system by oxidation with OH and RO\(_2\) radicals; while \( t_{1/2} = 7.3 \) d based on rate constant \( k = 3 \times 10^5 \) M\(^{-1}\) 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

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<tr>
<th>Stull 1947</th>
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<th>Forziati et al. 1950</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
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<th>( t/°C )</th>
<th>( P/Pa )</th>
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<td>–17.92</td>
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<td>12.8</td>
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<td>40.359</td>
<td>143295</td>
<td>–9.789</td>
<td>19998</td>
<td>–9.789</td>
<td>19998</td>
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<td>30.1</td>
<td>101325</td>
<td>45.614</td>
<td>169079</td>
<td>1.368</td>
<td>33331</td>
<td>–3.640</td>
<td>26664</td>
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<td>mp/°C</td>
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<td>50.914</td>
<td>198557</td>
<td>1.368</td>
<td>33331</td>
<td>12.664</td>
<td>53329</td>
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<tr>
<td>56.253</td>
<td>232061</td>
<td>eq. 2</td>
<td>P/mmHg</td>
<td>5.624</td>
<td>39997</td>
<td>18.416</td>
<td>66661</td>
</tr>
<tr>
<td>61.641</td>
<td>270071</td>
<td>A</td>
<td>6.78568</td>
<td>12.664</td>
<td>53329</td>
<td>23.319</td>
<td>79993</td>
</tr>
<tr>
<td></td>
<td></td>
<td>B</td>
<td>1014.294</td>
<td>18.416</td>
<td>66661</td>
<td>23.319</td>
<td>79993</td>
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<td></td>
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<td>C</td>
<td>229.783</td>
<td>23.319</td>
<td>79993</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \Delta H_f/(kJ \cdot mol^{-1}) = )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>at 25°C</td>
<td>25.47</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>at bp</td>
<td>25.20</td>
<td></td>
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</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.29</td>
<td>1.995</td>
</tr>
<tr>
<td>30.3</td>
<td>1.852</td>
</tr>
<tr>
<td>40.4</td>
<td>1.740</td>
</tr>
<tr>
<td>50.28</td>
<td>1.630</td>
</tr>
</tbody>
</table>

FIGURE 2.1.2.1.6.2 Logarithm of $K_{OA}$ versus reciprocal temperature for 1-pentene.
2.1.2.1.7 cis-2-Pentene

Common Name: cis-2-Pentene
Synonym: (Z)-2-pentene
Chemical Name: cis-2-pentene
CAS Registry No: 627-20-3
Molecular Formula: C₅H₁₀
Molecular Weight: 70.133
Melting Point (°C):
-151.36 (Lide 2003)
Boiling Point (°C):
36.93 (Lide 2003)
Density (g/cm³ at 20°C):
0.6556, 0.6504 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
107.0, 107.8 (20°C, 25°C, calculated-density)
111.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₐₜ (kJ/mol):
7.112 (Riddick et al. 1986)
7.11 (Chickos et al. 1999)
Entropy of Fusion, ΔSₘₐₜ (J/mol K):
58.39, 52.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
203 (shake flask-GC, cis-trans form not specified, McAuliffe 1966)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):  
log (P/mmHg) = 6.87540 – 1069.460/(240.786 + t°C); temp range 1.595–68.842°C (Antoine eq., ebulliometric method, Scott & Waddington 1950)
65940 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.87274 – 1068.0/(231.0 + t°C); temp range –33 to 82°C (Antoine eq. for liquid state, Dreisbach 1959)
66000, 65941 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.87274 – 1067.951/(230.585 + t°C); temp range –48.7 to 58.31°C (Antoine eq., Zwolinski & Wilhoit 1971)
65950 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.99984 – 1069.227/(230.757 + t°C); temp range 1.595–68.88°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 (P/kPa) = 5.96798 – 1052.44/(228.693 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P/mmHg) = 6.84308 – 1052.44/(228.69 + t°C); temp range –49 to 58°C (Antoine eq., Dean 1985, 1992)
65970 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 5.99069 – 1064.178/(-43.035 + T/K); temp range 234–318 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 34.0427 – 2.4524 × 10⁵/(T/K) – 9.5014 log (T/K) – 5.0816 × 10⁻¹¹·(T/K) + 4.3638 × 10⁻⁶·(T/K)²; temp range 122–476 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
22800  (calculated-P/C, Mackay & Shiu 1981)
22770  (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log $K_{ow}$:
2.20  (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 $K_{oa}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
- $k_{O(3P)} = 1.80 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with O(3P) atom (Herron & Huie 1973; quoted, Gaffney & Levine 1979)
- $k_{OH} = 6.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)
- $k_{OH} = (6.23 \pm 0.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Ohta 1984)
- $k_{OH} = (65.4 - 65.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298–303 K (Atkinson 1989)
- $k_{OH} = 6.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)
- $k_{OH} = 6.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an estimated atmospheric lifetime of 2.29 h in summer daylight (Altshuller 1991)
- $k_{OH} = 6.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O(3P)} = 1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with O(3P) atom at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation reaction rate constant $k = 6.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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: $t_\frac{1}{2} \approx 320 \text{ h}$ for oxidation by OH radicals, $t_\frac{1}{2} = 9 \times 10^4 \text{ d}$ for olefins in aquatic system, and $t_\frac{1}{2} = 7.3 \text{ d}$ based on rate constant $k = 3 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ 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 1950

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.595</td>
<td>25009</td>
<td>58.070</td>
<td>198556</td>
</tr>
<tr>
<td>6.522</td>
<td>31163</td>
<td>63.456</td>
<td>232087</td>
</tr>
<tr>
<td>11.486</td>
<td>38546</td>
<td>68.882</td>
<td>270057</td>
</tr>
<tr>
<td>16.494</td>
<td>47357</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21.541</td>
<td>57795</td>
<td>log ( P = A - B/(C + t/°C) )</td>
<td></td>
</tr>
<tr>
<td>26.633</td>
<td>70102</td>
<td>bp/°C</td>
<td>36.94</td>
</tr>
<tr>
<td>31.766</td>
<td>84518</td>
<td></td>
<td>P/mmHg</td>
</tr>
<tr>
<td>36.944</td>
<td>101329</td>
<td>A</td>
<td>6.87540</td>
</tr>
<tr>
<td>42.161</td>
<td>120804</td>
<td>B</td>
<td>1069.460</td>
</tr>
<tr>
<td>47.423</td>
<td>143281</td>
<td>C</td>
<td>240.786</td>
</tr>
<tr>
<td>52.724</td>
<td>169066</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
2.1.2.1.8 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: C₆H₁₂; CH₃(CH₂)₂C(CH₃)CH₂
Molecular Weight: 84.159

Melting Point (°C):
–135.7 (Dreisbach 1959; Lide 2003)

Boiling Point (°C):
60.7 (Dreisbach 1959)
62.1 (Lide 2003)

Density (g/cm³ at 20°C):
0.6799, 0.6751 (20°C, 25°C, Dreisbach 1959)

Molar Volume (cm³/mol):
123.8, 124.7 (20°C, 25°C, calculated-density)
133.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔHₜₜ (kJ/mol):

Entropy of Fusion, ΔSₜₜ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equations):
27464 (calculated-Antoine eq., Dreisbach 1959)

\[
\log (P/\text{mmHg}) = 6.88772 – 1154.7/(227.0 + t/°C); \text{ temp range } -14 \text{ to } 100°C \text{ (Antoine eq. for liquid state, Dreisbach 1959)}
\]

26000, 26051 (interpolated-Antoine eq., derived from compiled data, Zwolinski & Wilhoit 1971)

\[
\log (P/\text{mmHg}) = 6.85030 – 1138.516/(224.764 + t/°C); \text{ temp range } -30.1 \text{ to } 85.16°C \text{ (Antoine eq., Zwolinski & Wilhoit 1971)}
\]

\[
\log (P/\text{mmHg}) = 5.99434 – 1148.616/(–49.853 + T/K); \text{ temp range: } 275–344 K \text{ (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{mmHg}) = 32.9509 – 2.8171 \times 10^3/(T/K) – 8.9572 \times 10^{11}/(T/K) + 3.1710 \times 10^6/(T/K)^2; \text{ temp range } 137–507 K \text{ (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C):
28100 (calculated-P/C, Mackay & Shiu 1981)
28093 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log $K_{OW}$:

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
  - $k_{O3} = 1.05 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ under atmospheric conditions (Atkinson & Carter 1984)
  - $k_{OH} = (8.76 \pm 0.14) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 $\pm$ 2 K (relative rate method, Ohta 1984)
  - $k_{OH} = 62.6 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1985, Atkinson 1989)
  - $k_{OH} = 6.3 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{O3} = 15.0 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
- Surface water: $t_{1/2} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 8.0$ d, based on rate constant $k = 1.0 \times 10^6$ M$^{-1}$ 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: C₆H₁₂
Molecular Weight: 84.159
Melting Point (°C):
-153.6 (Dreisbach 1959; Lide 2003)
Boiling Point (°C):
53.88 (Dreisbach 1959)
53.9 (Lide 2003)
Density (g/cm³ at 20°C):
0.6642, 0.6594 (20°C, 25°C, Dreisbach 1059)
Molar Volume (cm³/mol):
126.7 (20°C, calculated-density, McAuliffe 1966, Ruelle & Kesselring 1997)
127.6 (25°C, calculated-density)
133.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
48.0 (shake flask-GC, McAuliffe 1966)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
35600 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.87757 – 1130.0/(229.0 + t/°C); temp range –20 to 91°C (Antoine eq. for liquid state, Dreisbach 1959)
36104, 36100 (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.83529 – 1121.302/(229.687 + t/°C); temp range –37.5 to 76.75°C (Antoine eq., Zwolinski & Wilhoit 1971)
36110 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 44.7746 – 2.7364 × 10⁻³(T/K) – 14.283·log (T/K) + 7.31 × 10⁻³·(T/K) + 4.8402 × 10⁻¹⁴·(T/K)²; temp range 120–496 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
62270 (calculated as 1/K_{AW}, C₆H₁₂/C₆H₁₂, 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 K_{ow}:
2.50 (calculated-π constant, Hansch et al. 1968)
2.51 (calculated-MCI χ, Murray et al. 1975)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{O3} = 1.06 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson & Carter 1984)
- $k_{O3} = 9.2 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

- Surface water: $t_{1/2} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 8.0$ d, based on rate constant $k = 1.0 \times 10^6$ M$^{-1}$ s$^{-1}$ for oxidation of substituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985).
2.1.2.1.10 1-Hexene

<table>
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<tr>
<th>Common Name: 1-Hexene</th>
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<tbody>
<tr>
<td>Synonym: α-hexene</td>
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<tr>
<td>Chemical Name: 1-hexene</td>
</tr>
<tr>
<td>CAS Registry No: 646-04-8</td>
</tr>
<tr>
<td>Molecular Formula: C₆H₁₂; CH₃(CH₂)₃CHCH₂</td>
</tr>
<tr>
<td>Molecular Weight: 84.159</td>
</tr>
<tr>
<td>Melting Point (°C):</td>
</tr>
<tr>
<td>-139.76 (Lide 2003)</td>
</tr>
<tr>
<td>Boiling Point (°C):</td>
</tr>
<tr>
<td>63.48 (Lide 2003)</td>
</tr>
<tr>
<td>Density (g/cm³ at 20°C):</td>
</tr>
<tr>
<td>0.6732, 0.6685 (20°C, 25°C, Forzati et al. 1950; Dreisbach 1959; Riddick et al. 1986)</td>
</tr>
<tr>
<td>Molar Volume (cm³/mol):</td>
</tr>
<tr>
<td>125.0 (20°C, calculated-density, McAuliffe 1966; Wang et al. 1992; Ruelle &amp; Kesselring 1997)</td>
</tr>
<tr>
<td>125.9 (25°C, calculated-density)</td>
</tr>
<tr>
<td>133.2 (calculated-Le Bas method at normal boiling point, Eastcott et al. 1988)</td>
</tr>
<tr>
<td>Enthalpy of Fusion, ΔHᶠus (kJ/mol):</td>
</tr>
<tr>
<td>9.347 (Riddick et al. 1986)</td>
</tr>
<tr>
<td>9.35 (Chickos et al. 1999)</td>
</tr>
<tr>
<td>Entropy of Fusion, ΔSᶠus (J/mol K):</td>
</tr>
<tr>
<td>70.1, 61.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)</td>
</tr>
<tr>
<td>Fugacity Ratio at 25°C, F: 1.0</td>
</tr>
<tr>
<td>Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):</td>
</tr>
<tr>
<td>50.0 (shake flask-GC, McAuliffe 1966)</td>
</tr>
<tr>
<td>65.5 (shake flask-titration, Natarajan &amp; Venkatachalam 1972)</td>
</tr>
<tr>
<td>65.5, 54.12, 42.16 (25, 30, 35°C, shake flask-titration, in 0.001M HNO₃ solution, Natarajan &amp; Venkatachalam 1972)</td>
</tr>
<tr>
<td>55.4 (shake flask-GC, Leinonen &amp; Mackay 1973)</td>
</tr>
<tr>
<td>60.0 (20°C, shake flask-GC, Budantseva et al. 1976)</td>
</tr>
<tr>
<td>69.7 (generate column-GC, Tewari et al. 1982a)</td>
</tr>
<tr>
<td>100, 53 (20°C, 25°C, “best” values, IUPAC Solubility Data Series, Shaw 1989a)</td>
</tr>
<tr>
<td>In x = −268.791 + 11353.70/(T/K) + 38.4871·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsopouloous 2001)</td>
</tr>
<tr>
<td>In x = −276.423 + 11833.54/(T/K) + 39.5126·ln (T/K); temp range 290–400 K (eq. derived from direct fit of solubility data, Tsopouloous 2001)</td>
</tr>
<tr>
<td>51.43* (calculated-liquid-liquid equilibrium LLE data, temp range 293.2–494.3 K, Góral et al. 2004)</td>
</tr>
<tr>
<td>Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):</td>
</tr>
<tr>
<td>22300* (Antoine eq. regression, temp range −57.5 to 66°C, Stull 1947)</td>
</tr>
<tr>
<td>23500* (23.7°C, ebulliometry-manometer, measured range 15.9–64.3°C, Forzati et al. 1950)</td>
</tr>
<tr>
<td>log (P/mmHg) = 6.86573 − 1152.971/(225.849 + t°C); temp range 15.9–64.3°C (Antoine eq., ebulliometry-manometer measurements, Forzati et al. 1950)</td>
</tr>
<tr>
<td>25000 (calculated-Antoine eq., Dreisbach 1959)</td>
</tr>
<tr>
<td>log (P/mmHg) = 6.86572 − 1152.971/(226.0 + t°C); temp range −12 to 79°C (Antoine eq. for liquid state, Dreisbach 1959)</td>
</tr>
<tr>
<td>24800*, 24798 (interpolated-Antoine eq., derived from compiled data, Zwolinski &amp; Wilhoit 1971)</td>
</tr>
<tr>
<td>log (P/mmHg) = 6.86573 − 1152.971/(225.849 + t°C); temp range −29.3 to 86.64°C (Antoine eq., Zwolinski &amp; Wilhoit 1971)</td>
</tr>
</tbody>
</table>
\[
\log (P/\text{mmHg}) = [-0.2185 \times 7787.6/(T/\text{K})] + 7.930324; \text{ temp range } -57.5 \text{ to } 66^\circ \text{C (Antoine eq., Weast 1972--73)}
\]

\[
24800 \text{ (interpolated-Antoine eq., Boublik et al. 1984)}
\]

\[
\log (P/\text{kPa}) = 5.98426 - 1154.952/(225.25 + t/°\text{C}); \text{ temp range } 15.89-64.311^\circ\text{C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublik et al. 1984)}
\]

\[
24800 \text{ (interpolated-Antoine eq., temp range } -16 \text{ to } 64^\circ\text{C, Dean 1985, 1992)}
\]

\[
\log (P/\text{mmHg}) = 6.85770 - 1148.62/(225.346 + t/°\text{C}); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]

\[
24800 \text{ (interpolated-Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{kPa}) = 5.98260 - 1154.952/(226.002 + t/°\text{C}); \text{ temp range } -16 \text{ to } 64^\circ\text{C (Antoine eq., Dean 1985, 1992)}
\]

\[
24800 \text{ (interpolated-Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{mmHg}) = 33.4486 - 2.6221 \times 10^3/(T/\text{K}) - 9.1784 \times 10^{-12} \times (T/\text{K}) + 3.093 \times 10^{-6} \times (T/\text{K})^2; \text{ temp range } 133-504 \text{ K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa m²/mol at 25°C):

\[
41750 \text{ (calculated-P/C, Mackay & Shiu 1975)}
\]

\[
44080 \text{ (calculated-1/KAW, CW/CA, reported as exptl., Hine & Mookerjee 1975)}
\]

\[
51790, 34220 \text{ (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)}
\]

\[
41800 \text{ (calculated-P/C, Mackay & Shiu 1981)}
\]

\[
47230 \text{ (calculated- } \chi, \text{ Nirmalakhandan & Speece 1988)}
\]

\[
41640 \text{ (calculated-P/C, Eastcott et al. 1988)}
\]

\[
29940 \text{ (calculated-vapor–liquid equilibrium (VLE) data, Yaws et al. 1991)}
\]

Octanol/Water Partition Coefficient, log K\text{OW:}:

\[
3.39 \text{ (generator column-GC, Tewari et al. 1982a,b)}
\]

\[
3.47 \text{ (calculated-activity coeff. } \gamma, \text{ Wasik et al. 1981)}
\]

\[
3.48 \text{ (calculated-activity coeff. } \gamma, \text{ Wasik et al. 1982)}
\]

\[
3.39, 3.40 \text{ (generator column-GC, calculated-activity coeff. } \gamma, \text{ Schantz & Martire 1987)}
\]

\[
3.40 \text{ (recommended, Sangster 1989)}
\]

\[
3.39 \text{ (recommended, Hansch et al. 1995)}
\]

Octanol/Air Partition Coefficient, log K\text{OA} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

\[
2.50* \text{ (20.29°C, from GC-determined } \gamma^\infty \text{ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)}
\]

\[
2.41 \text{ (calculated-measured } \gamma^\infty \text{ in pure octanol and vapor pressure P, Abraham et al. 2001)}
\]

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K\text{OC:}:

Environmental Fate Rate Constants, k, and Half-Lives, t\text{½:}

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k\text{OH} for reaction with OH radical, k\text{NO3} with NO3 radical and k\text{O3} with O3 or as indicated, *data at other temperatures see reference:

\[
k\text{O3} = 0.90 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Cadle & Schadt 1952)}
\]

\[
k\text{O3} = 1.00 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Hanst et al. 1958)}
\]

\[
k\text{O3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 30^\circ\text{C (flow system, Bifulini & Altshuller 1965)}
\]

\[
k\text{O3} = 1.40 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (static system-chemiluminescence, Cox & Penkett 1972)}
\]

\[
k\text{O3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \text{ K (static system-chemiluminescence, Stedman et al. 1973)}
\]

\[
k\text{O3} = 1.11 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (static system-chemiluminescence, Japar et al. 1974)}
\]

\[
k\text{O3} = 1.08 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 294 \pm 2 \text{ K (static system-chemiluminescence, Adeniji et al. 1981)}
\]

\[
k\text{O3} = 1.21 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K (static system-chemiluminescence, Atkinson et al. 1982)}
\]

\[
k\text{O3} = (0.91 \text{ to } 1.36) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 294-303 \text{ K (Atkinson & Carter 1984)}
\]

\[
k\text{OH} = 3.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K (relative rate method, Atkinson & Aschmann 1984)}
\]
Aliphatic and Cyclic Hydrocarbons

\[ k_{OH} = (3.75 - 3.25) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295-303 \text{ K (Atkinson 1985)} \]
\[ k_{OH} = (32.9 - 37.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295-303 \text{ K (Atkinson 1989)} \]
\[ k_{OH} = 3.18 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{O_3} = 1.17 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1990)} \]
\[ k_{O_3} = 1.10 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1997)} \]
\[ k_{OH} = 3.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{O_3} = 11.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ and } k_{O(3P)} = 4.65 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O(3P) atom at } 298 \text{ K (recommended, Atkinson 1997)} \]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: \( t_{1/2} \sim 320 \text{ h and } 9 \times 10^4 \text{ d for oxidation by OH and RO}_2 \text{ radicals for olefins in aquatic system, and } t_{1/2} = 7.3 \text{ d, based on rate constant } k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \text{ for oxidation of unsubstituted olefins with singlet oxygen in aquatic system (Mill & Mabey 1985)} \).

<table>
<thead>
<tr>
<th>Table 2.1.2.1.10.1</th>
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<tr>
<td><strong>Reported aqueous solubilities of 1-hexene at various temperatures</strong></td>
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<td>20</td>
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<td>25</td>
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<td>36.8</td>
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**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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\ln P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\ln P &= A - B/(C + t/°C) \\
\log P &= A - B/(T/K) - C \cdot \log(T/K)
\end{align*}
\]

<table>
<thead>
<tr>
<th>Stull 1947</th>
<th>Forziati et al. 1950</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
<th>Selected values</th>
<th>GC det’d activity coefficient</th>
</tr>
</thead>
<tbody>
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<td>(t/°C)</td>
<td>(P/Pa)</td>
<td>(t/°C)</td>
<td>(P/Pa)</td>
<td>(t/°C)</td>
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<td>64.311</td>
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<td>50.859</td>
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<td>50.859</td>
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<td>64.311</td>
<td>103995</td>
<td>44.569</td>
<td>53329</td>
<td>50.859</td>
</tr>
<tr>
<td>(\Delta H_f/(kJ \text{ mol}^{-1}))</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>at 25°C</td>
<td>28.28</td>
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<td>at bp</td>
<td>30.63</td>
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</tr>
</tbody>
</table>

\(\Delta H_f\) is the enthalpy of formation.
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 $K_{OA}$ versus reciprocal temperature for 1-hexene.
2.1.2.1.11 1-Heptene

Common Name: 1-Heptene
Synonym: 1-heptylene, α-heptene
Chemical Name: 1-heptene
CAS Registry No: 592-76-7
Molecular Formula: C\textsubscript{7}H\textsubscript{14}, CH\textsubscript{3}(CH\textsubscript{2})\textsubscript{4}CH=CH\textsubscript{2}
Molecular Weight: 98.186
Melting Point (°C):
-118.9  (Lide 2003)
Boiling Point (°C):
93.64  (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.6970, 0.6927  (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959)
Molar Volume (cm\textsuperscript{3}/mol):
140.9  (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
141.8  (25°C, calculated-density)
155.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
35.65, 31.09 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{ fus}\) (kJ/mol):
12.401 (Riddick et al. 1986)
12.66  (Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):
82.5, 77.5  (exp., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
31.03, 27.6, 24.06 (20°C, 25°C, 30°C, shake flask-titration, in 0.001M HNO\textsubscript{3} solution, Natarajan & Venkatachalam 1972)
18.16  (generator column-GC, Tewari et al. 1982a)
23.6  (calculated-activity coeff. \(\gamma\) and \(K_{ow}\), Tewari et al. 1982b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
7690*  (25.5°C, ebulliometry-manometer, measured range 21.6–94.5°C, Forziati et al. 1950)
log (P/mmHg) = 6.90069 – 1257.505/(219.179 + t\textdegree C); temp range 21.6–94.5°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
7510  (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.90069 – 1257.505/(219.18 + t\textdegree C); temp range 10–128°C (Antoine eq. for liquid state, Dreisbach 1959)
7506*, 7510  (derived from compiled data, interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.90069 – 1257.505/(219.179 + t\textdegree C); temp range –6.07 to 118.44°C (Antoine eq. eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 8643.2/(T/K)] + 7.991519; temp range –35.8 to 98.5°C (Antoine eq., Weast 1972–73)
7520, 7530  (interpolated-Antoine equations., Boublík et al. 1984)
log (P/kPa) = 6.04107 – 1266.473/(220.202 + t\textdegree C); temp range 21.6–94.53°C (Antoine eq. from reported expvl. data of Forziati et al. 1950, Boublík et al. 1984)
Aliphatic and Cyclic Hydrocarbons

\[ \log (P \text{/kPa}) = 6.03512 - \frac{1263.343}{219.922 + \frac{t}{\text{°C}}}; \text{temp range 54.17–93.61°C} \ (\text{Antoine eq. from reported exptl. data, Boublik et al. 1984}) \]

7515 \ (\text{interpolated-Antoine eq., Dean 1985, 1992})

\[ \log (P \text{/mmHg}) = 6.91087 - \frac{1258.345}{219.30 + \frac{t}{\text{°C}}}; \text{temp range –6 to 118°C} \ (\text{Antoine eq., Dean 1985, 1992}) \]

7500 \ (\text{quoted lit., Riddick et al. 1986})

\[ \log (P \text{/kPa}) = 6.02677 - \frac{1258.34}{219.299 + \frac{t}{\text{°C}}}; \text{temp range not specified} \ (\text{Antoine eq., Riddick et al. 1986}) \]

7500 \ (\text{extrapolated-Antoine eq., Stephenson & Malanowski 1987})

\[ \log (P \text{/kPa}) = 5.99079 - \frac{1237.44}{-56.26 + \frac{T}{\text{K}}}; \text{temp range 311–368 K} \ (\text{Antoine eq., Stephenson & Malanowski 1987}) \]

\[ \log (P \text{/mmHg}) = 38.1255 - 3.064 \times 10^{3}/(T/\text{K}) - 10.679 \cdot \log (T/\text{K}) + 1.2244 \times 10^{-10} \cdot (T/\text{K})^{2}; \text{temp range 154–537 K} \ (\text{vapor pressure eq., Yaws 1994}) \]

Henry’s Law Constant (Pa m^3/mol at 25°C):

40580 \ (\text{calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991})

Octanol/Water Partition Coefficient, log \( K_{ow} \):

3.99 \ (\text{generator column-concn. ratio-GC, Tewari et al. 1982a,b})

4.09 \ (\text{calculated-activity coeff. \( \gamma \), Wasik et al. 1982})

4.06 \ (\text{generator column-GC, Schantz & Martire 1987})

3.99 \ (\text{recommended, Sangster 1989, 1993})

3.99 \ (\text{recommended, Hansch et al. 1995})

Octanol/Air Partition Coefficient, log \( K_{oa} \):

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{oc} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO_3 radical and \( k_{O3} \) with O_3 or as indicated, *data at other temperatures see reference:

\[
\begin{align*}
k_{O3} &= 8.1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \ (\text{Cadle & Schadt 1952}) \\
k_{O3} &= 1.73 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K} \ (\text{static system-chemiluminescence, Atkinson et al. 1982}) \\
k_{OH} &= 3.97 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 K} \ (\text{relative rate method, Atkinson & Aschmann 1984}) \\
k_{OH} &= 40.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } 36.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K and 305 K respectively} \ (\text{Atkinson 1989}) \\
k_{OH} &= 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{O3} = 1.73 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \ (\text{Atkinson 1990}) \\
k_{OH} &= 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{O3} = 12.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \ (\text{recommended, Atkinson 1997}) \\
\end{align*}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: \( t_{1/2} \approx 320 \text{ h} \) and \( 9 \times 10^4 \text{ d} \) for oxidation by OH and RO_2 radicals for olefins in aquatic system, and \( t_{1/2} = 7.3 \text{ d} \), based on rate constant \( k = 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1} \) 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

\[
\log P = A - \frac{B}{T} (K) \\
\log P = A - \frac{B}{C + t/°C} \\
\log P = A - \frac{B}{C + T/K} \\
\log P = A - \frac{B}{T/K} - C \log (T/K)
\]

(1) \quad \ln P = A - \frac{B}{T} (1a)

Forziati et al. 1950

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Eubulliometry

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Eisen & Orav 1970

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Zwolinski & Wilhoit 1971

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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: α-octene, caprylene, α-octylene
Chemical Name: 1-octene
CAS Registry No: 111-66-0
Molecular Formula: C₈H₁₆; CH₃(CH₂)₅CH=CH₂
Molecular Weight: 112.213
Melting Point (°C): –101.7 (Lide 2003)
Boiling Point (°C): 121.29 (Lide 2003)
Density (g/cm³ at 20°C):
0.7149, 0.7109 (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
154.9 (20°C, calculated-density, Stephenson & Malanowski 1987)
177.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
40.35, 33.95 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
15.569 (Riddick et al. 1986)
15.31 (Chickos et al. 1999)
Entropy of Fusion, ΔSₘₙ (J/mol K):
89.29, 86.8 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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. γ and KOW, Tewari et al. 1982b)
2.70, 22.2 (quoted, IUPAC Solubility Data Series, Shaw 1989)
2.93, 2.93 (25, 37.78°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
6382* (44.893°C, ebulliometry, measured range 44.893–122.223°C, Forziati et al. 1950)
log (P/mmHg) = 6.93262 – 1353.486/(212.765 + t°C); temp range 44.8–122.2°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
2317 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.93263 – 1253.5/(212.764 + t°C); temp range 0–151°C (Antoine eq. for liquid state, Dreisbach 1959)
2320* (interpolated-Antoine eq., temp range 15.38–147.54°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.93263 – 1253.486/(212.764 + t°C); temp range 15.38–147.54°C (Antoine eq., Zwolinski & Wilhoit 1971)
2320 (extrapolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 6.06421 – 1356.472/(213.099 + t°C); temp range 44.89–122.2°C (Antoine eq. from reported exptl. data Forziati et al. 1950, Boublík et al. 1984)
2320 (interpolated-Antoine eq., temp range 15–147°C, Dean 1985, 1992)
log (P/mmHg) = 6.93495 – 1355.46/(213.05 + t°C); temp range 15–147°C (Antoine eq., Dean 1985, 1992)
2300 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 6.05985 – 1355.46/(213.054 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
2320 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.05178 – 1350.245/(–60.716 + T/K); temp range 317–400 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 56.1183 – 3.7657 × 10³/(T/K) – 10.006·log (T/K) + 7.7387 × 10⁻³·(T/K) – 1.3036 × 10⁻⁶·(T/K)²; temp range 171–567 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

91700 (calculated-P/C, Mackay & Shiu 1975; selected, Mills et al. 1982)
96440 (calculated-1/KAW, CW/CA, 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 χ, Nirmalakhandan & Speece 1988)
65500 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log KOW:

4.57 (generator column-GC, Tewari et al. 1982a)
4.56, 4.72 (generator column-GC, calculated-activity coeff. γ, Schantz & Martire 1987)
4.57 (recommended, Sangster 1989)
4.57 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log KOA:

3.53 (calculated-measured γ∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log KOC:

Environmental Fate Rate Constants, k, and Half-Lives, t½:

Volatilization:

Photolysis:

Oxidation: rate constant k; for gas-phase second-order rate constants, kOH for reaction with OH radical, kNO₃ with NO₃ radical and kO₃ with O₃ or as indicated, *data at other temperatures see reference:
kO₃ = 8.1 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ for the reaction with ozone in air (Atkinson & Carter 1984)
kOH = 4.0 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, kO₃ = 1.70 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹, and kO₃[O(3P)] = 1.10 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with O(3P) atom in gas phase (Paulson & Seinfeld 1992)
kO₃ = 14.0 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: t½ ~ 320 h and 9 × 10⁴ d for oxidation by OH and RO₂ radicals for olefins in aquatic system, and t½ ~ 7.3 d, based on rate constant k = 3 × 10³ M⁻¹ 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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C \log (T/K)
\end{align*}
\]

\[\text{Forziati et al. 1950} \]

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\[\text{Zwolinski & Wilhoit 1971} \]

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\[\Delta H_v/(kJ mol^{-1}) = 106.997\]  

FIGURE 2.1.2.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for 1-octene.
2.1.2.1.13 1-Nonene

Common Name: 1-Nonene
Synonym: α-nonene, n-heptylene, 1-nonylene
Chemical Name: 1-nonene
CAS Registry No: 124-11-8
Molecular Formula: C₉H₁₈; CH₃(CH₂)₆CH=CH₂
Molecular Weight: 126.239
Melting Point (°C): –81.3 (Lide 2003)
Boiling Point (°C): 146.9 (Lide 2003)
Density (g/cm³ at 20°C):
0.7292, 0.7235 (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959; Riddick et al. 1986)
Molar Volume (cm³/mol):
173.1, 174.1 (20°C, 25°C, calculated-density)
199.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
45.52, 36.31 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
19.075 (Riddick et al. 1986)
19.37 (Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
104.23, 96.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.63 (estimated-nomograph, Brookman et al. 1986)
1.12 (generator column-GC, Tewari et al. 1982a)
2.09 (calculated-activity coeff. γ and KOW, Tewari et al. 1982b)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
6385* (66.60°C, ebulliometry, measured range 66.607–147.860°C, Forziati et al. 1950)
log (P/mmHg) = 6.95389 – 1435.359/(205.535 + t°C); temp range 66.6–147.9°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
712 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.95387 – 1435.295/(205.535 + t°C); temp range 25–173°C (Antoine eq. for liquid state, Dreisbach 1959)
707*, 712 (derived from compiled data, extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.95430 – 1436.20/(205.69 + t°C); temp range 35–175°C (Antoine eq., Dean 1985, 1992)
710 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 6.07920 – 1436.20/(205.690 + t/K); temp range not specified (Antoine eq., Riddick et al. 1986) 712 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.07341 – 1432.435/(–67.884 + T/K); temp range 339–423 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 60.6089 – 4.2023 × 10³/(T/K) – 19.446·log (T/K) + 7.8308 × 10⁻³·(T/K)²; temp range 192–593 K (vapor pressure eq., Yaws 1994)
650.4 (23.25°C, transpiration method, Verevkin et al. 2000)
ln (P/Pa) = 24.60 – 5379/(T/K); temp range 278.5–318.3 K (transpiration method, Verevkin et al. 2000)
Henry’s Law Constant (Pa m³/mol at 25°C):
80450  (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 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 $K_{oa}$:
- 3.83  (calculated-measured $\gamma^{-}$ in pure octanol and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{oc}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:
Surface water: $t_{1/2} \approx 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 7.3$ d, based on rate constant $k = 3 \times 10^3$ M$^{-1}$ 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

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Forziati et al. 1950

Zwolinski & Wilhoit 1971

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<td>78.651</td>
<td>10666</td>
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<td>P/mmHg</td>
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<td>84.210</td>
<td>13332</td>
<td>A</td>
<td>6.95387</td>
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<tr>
<td>94.889</td>
<td>19998</td>
<td>B</td>
<td>1435.359</td>
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<td>102.956</td>
<td>26664</td>
<td>C</td>
<td>205.535</td>
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<td>109.518</td>
<td>33331</td>
<td>bp/°C</td>
<td>146.868</td>
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<td>115.090</td>
<td>39997</td>
<td>$\Delta H_v/(kJ \text{ mol}^{-1})$ =</td>
<td></td>
</tr>
<tr>
<td>124.295</td>
<td>53329</td>
<td>at 25°C</td>
<td>36.32</td>
</tr>
<tr>
<td>131.808</td>
<td>66661</td>
<td>at bp</td>
<td>45.52</td>
</tr>
<tr>
<td>138.204</td>
<td>79993</td>
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</tbody>
</table>
FIGURE 2.1.2.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for 1-nonene.
2.1.2.1.14 1-Decene

Common Name: 1-Decene
Synonym: α-decene
Chemical Name: 1-decene
CAS Registry No: 872-05-9
Molecular Formula: C_{10}H_{20}
Molecular Weight: 140.266
Melting Point (°C):
-66.3 (Lide 2003)
Boiling Point (°C):
170.5 (Lide 2003)
Density (g/cm³ at 20°C):
0.7408, 0.7369 (20°C, 25°C, Forziati et al. 1950; Dreisbach 1959)
Molar Volume (cm³/mol):
189.3 (20°C, calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
190.3 (25°C, calculated-density)
222.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
50.43, 38.66 (25°, bp, Riddick et al. 1986)
Enthalpy of Fusion, ΔHfus (kJ/mol):
21.75 (Chickos et al. 1999)
Entergy of Fusion, ΔSfus (J/mol K):
106.8, 105.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
5.70 (shake flask-titration with bromine, Natarajan & Venkatachalam 1972; quoted Shaw 1989)
11.0, 8.50, 5.70 (15, 20, 25°C, shake flask-titration, in 0.001M HNO₃ solution, Natarajan & Venkatachalam 1972)
0.161 (calculated-K_{OP}, Wang et al. 1992)
0.433 (calculated-molar volume Vₘ, 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 (101, 151.5, 202°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°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* (14.7°C, summary of literature data, temp range 14.7–192.0°C, Stull 1947)
6997* (86.774°C, ebulliometry, measured range 86.774–171.605°C, Forziati et al. 1950)
log (P/mmHg) = 6.96036 – 1501.812/(197.578 + t/°C); temp range 86.7–171.6°C (Antoine eq., ebulliometry-manometer measurements, Forziati et al. 1950)
218 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 6.96034 – 1501.872/(197.58 + t/°C); temp range 25–253°C (Antoine eq. for liquid state, Dreisbach 1959)
218* (extrapolated-Antoine eq., temp range 54.4–199.3°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.96034 – 1501.872/(197.58 + t/°C); temp range 54.4–199.3°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/kPa) = 6.07985 – 1497.943/(197.102 + t/°C); temp range 86.7–171.6°C (Antoine eq. from reported exptl. data of Forziati et al. 1950, Boublík et al. 1984)
215 (extrapolated-Antoine eq., temp range: 54–199°C, Dean 1985, 1992)
log (P/mmHg) = 6.93477 – 1484.98/(195.707 + t/°C), temp range: 54–199°C (Antoine eq., Dean 1985, 1992)
210 (quoted lit., Riddick et al. 1986)
log (P/kPa) = 6.05967 – 1484.98/(195.707 + t°C); temp range not specified (Antoine eq., Riddick et al. 1986)
log (P1/kPa) = 6.12458 – 1528.811/(–72.566 + T/K); temp range 383–445 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 2.2678 – 3.1244 × 10³/(T/K) + 5.432·log (T/K) – 2.0137 × 10⁻²·(T/K) + 1.1221 × 10⁻⁵·(T/K)²; temp range 207–617 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{ow}:
   4.78 (calculated-regression eq. of Lyman et al. 1982, Wang et al. 1992)
   5.18 (calculated-molar volume V_M, Wang et al. 1992)
   4.7037 (calculated-UNIFAC group contribution, Chen et al. 1993)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{½}:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{oh} for reaction with OH radical, k_{no3}
with NO3 radical and k_{o3} with O3 or as indicated, #data at other temperatures see reference:
k_{o3} = 1.08 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ for reaction with ozone in the gas phase (Atkinson & Carter 1984)
k_{o3} = 9.3 × 10⁻¹⁸ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Surface water: t_{½} ~ 320 h and 9 × 10⁴ d for oxidation by OH and RO₂ radicals for olefins in aquatic system, and

TABLE 2.1.2.1.14.1
Reported vapor pressures of 1-decene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Summary of literature data</th>
<th>Forziati et al. 1950</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
</tr>
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<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
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<tr>
<td>14.7</td>
<td>133.3</td>
<td>133.3</td>
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<tr>
<td>40.3</td>
<td>666.6</td>
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(Continued)
### TABLE 2.1.2.14.1 (Continued)

<table>
<thead>
<tr>
<th>Stull 1947 summary of literature data</th>
<th>Forziati et al. 1950 ebulliometry</th>
<th>Zwolinski &amp; Wilhoit 1971 selected values</th>
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<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
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<tr>
<td>93.5</td>
<td>7999</td>
<td>106.223</td>
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<td>192.0</td>
<td>101325</td>
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<td>mebp/°C</td>
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<td>171.605</td>
<td>104026</td>
<td>171.605</td>
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<tr>
<td>mp/°C</td>
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</tbody>
</table>

eq. 2 \( P/\text{mmHg} \)
- A = 6.96036
- B = 1501.872
- C = 197.578

bp/°C = 170.5

\[ \Delta H_v/(\text{kJ mol}^{-1}) = \]
- at 25°C = 38.66
- at bp = 50.46

**FIGURE 2.1.2.14.1** 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: \(\text{C}_4\text{H}_6\); \(\text{CH}_2=\text{CHCH}=\text{CH}_2\)
Molecular Weight: 54.091
Melting Point (°C): 
-108.91 (Lide 2003)
Boiling Point (°C): 
-4.41 (Lide 2003)
Density (g/cm\(^3\) at 20°C): 
0.6211, 0.6149 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm\(^3\)/mol): 
87.1 (20°C, 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, \(\Delta H_{\text{fus}}\) (kJ/mol): 
7.98 (Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K): 
48.62, 45.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C): 
735 (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):

- 113857* (–1.50°C, static method-manometer, measured range –75.5 to –1.50°C, Heisig 1933)
- 336200* (calculated-Antoine eq. regression, temp range –102.8 to 4.6°C, Stull 1947)
- 280600 (calculated-Antoine eq., Dreisbach 1959)
- \(\log (P/\text{mmHg}) = 6.85941 - 935.53/(239.55 + t/\degree \text{C});\) temp range –66 to 46°C (Antoine eq. for liquid state, Dreisbach 1959)
- 281000* (extrapolated-Antoine eq., temp range –58.201 to 14.43°C, Zwolinski & Wilhoit 1971)
- 280644 (derived from compiled data, Zwolinski & Wilhoit 1971)
- \(\log (P/\text{mmHg}) = 6.84999 - 930.546/(238.854 + t/\degree \text{C});\) temp range –58.201 to 14.43°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 247700 (extrapolated-Antoine eq., temp range –82.5 to 9.7°C, Weast 1972–73)
- \(\log (P/\text{mmHg}) = [-0.2185 \times 7761.0/(T/\text{K})] + 8.997505;\) temp range –82.5 to 9.7°C (Antoine eq., Weast 1972–73)
- 281650, 281510* (static method quartz manometer, measured range 15–55°C, Flebbe et al. 1982)
- 281230, 310400 (extrapolated-Antoine equations, Boublík et al. 1984)
- \(\log (P/\text{kPa}) = 6.86369 - 1313.687/(275.492 + t/\degree \text{C});\) temp range –81 to –24°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
- \(\log (P/\text{mmHg}) = 5.97484 - 931.996/(239.329 + t/\degree \text{C});\) temp range –75 to –1.5°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
- \(\log (P/\text{mmHg}) = 7.03555 - 998.106/(245.233 + t/\degree \text{C});\) temp range –87 to –62°C (Antoine eq., Dean 1985, 1992)
- \(\log (P/\text{mmHg}) = 6.84999 - 930.546/(238.854 + t/\degree \text{C});\) temp range –58 to 15°C (Antoine eq., Dean 1985, 1992)
- 281000 (interpolated-Antoine eq.-III, Stephenson & Malanowski 1987)
\[
\log (P_{L}/kPa) = 6.16045 - 998.106/( -27.916 + T/K); \text{ temp range } 193\text{–}213 \text{ K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]
\[
\log (P_{L}/kPa) = 5.97489 - 930.546/( -34.306 + T/K); \text{ temp range } 213\text{–}276 \text{ K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]
\[
\log (P_{L}/kPa) = 5.99667 - 940.687/( -33.017 + T/K); \text{ temp range } 270\text{–}318 \text{ K (Antoine eq.-III, Stephenson & Malanowski 1987)}
\]
\[
\log (P_{L}/kPa) = 6.31615 - 1130.927/( -5.606 + T/K); \text{ temp range } 315\text{–}382 \text{ K (Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]
\[
\log (P_{L}/kPa) = 8.86984 - 3877.451/(315.612 + T/K); \text{ temp range } 380\text{–}425 \text{ K (Antoine eq.-V, Stephenson & Malanowski 1987)}
\]
\[
\log (P/\text{mmHg}) = 30.0572 - 1.9891 \times 10^{3}/(T/K) - 8.2922 \times \log (T/K) + 2.5664 \times 10^{-10} \times (T/K)^2; \text{ temp range } 164\text{–}425 \text{ K (vapor pressure eq., Yaws 1994)}
\]
\[
\ln (P/\text{atm}) = 9.16107 - 2154.139/(T/K - 33.596); \text{ temp range } 207\text{–}319 \text{ K (Antoine eq., Oliveira & Uller 1996)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C):

7460  \hspace{1em} (calculated-P/C, Mackay & Shiu 1981)

6370  \hspace{1em} (calculated-I/K_{AW}, C_{W/C_A}, reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1989)

7150, 6230  \hspace{1em} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

10820  \hspace{1em} (calculated-MCI \chi, Nirmalakhandan & Speece 1988)

7720  \hspace{1em} (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

1.99  \hspace{1em} (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979)

1.87, 1.68, 1.90  \hspace{1em} (calculated-fragment const., Rekker 1977)

2.22  \hspace{1em} (calculated-UNIFAC, Banerjee & Howard 1988)

1.99  \hspace{1em} (recommended, Sangster 1989)

1.56  \hspace{1em} (calculated-V_{M}, Wang et al. 1992)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

1.28  \hspace{1em} (calculated-K_{OW}, Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, log K_{OC}:

1.86–2.36  \hspace{1em} (soils and sediments, calculated-K_{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, k_{OH} for reaction with OH radical, k_{NO3} with NO\textsubscript{3} radical and k_{O(3P)} with O\textsubscript{(3P)} atom, or as indicated, \textsuperscript{*}data at other temperatures and/or the Arrhenius expression see reference:

\[
k_{O(3P)} = 8.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \text{ K (Japer et al. 1974)}
\]

\[
k_{OH} = (46.4 \pm 9.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at } 305 \pm 2 \text{ K (relative rate method, Lloyd et al. 1976)}
\]

\[
k_{OH} = 4.64 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}, t_{1/2} = 0.25 \text{ h for reaction with OH radical only, } t_{1/2} = 0.24 \text{ h with an average concn of 0.1 ppm of O}_{3} \text{ at 300 K (Darnall et al. 1976)}
\]

\[
k_{O_3} = 1.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O(P) atom at room temp. (Atkinson & Pitts, Jr. 1977)}
\]

\[
k_{OH}^{*} = (6.85 \pm 0.69) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299.5 \text{ K, measured range } 299.9\text{–}424 \text{ K (flash photolysis-resonance fluorescence, Atkinson et al. 1977)}
\]

\[
k_{OH} = 6.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson et al. 1979; quoted, Gaffney & Levine 1979)}
\]

\[
k_{O(3P)} = (1.17 \pm 0.19) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K, measured range } 276\text{–}324 \text{ K with atmospheric lifetime } \tau \sim 24 \text{ h due to reaction with O}_{3} \text{ and } \tau \sim 4 \text{ h with OH radical (Atkinson et al. 1982)}
\]
k_{OH} = 6.85 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 297 \pm K, \ k_{OH}^{(calc)} = 6.22 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (relative rate method, Ohta 1983)}

k_{O_3} = (6.1 - 8.4) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. to 299 K} \text{ (Atkinson & Carter 1984)}

k_{NO_3} = (5.34 \pm 0.62) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 K} \text{ (relative rate method, Atkinson et al. 1984a)}

k_{NO_2} = (3.1 \pm 0.3) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with NO}_2 \text{ at 295 \pm 2 K} \text{ (relative rate method, Atkinson et al. 1984b)}

k_{OH} = 6.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{NO_3} = 0.053 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{O_3} = 8.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \ k_{O(3P)} = 6.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{NO_2} = 3.1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with NO}_2 \text{ at room temp.} \text{ (Atkinson et al. 1984b)}

k_{OH} = 6.65 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 295 K} \text{ (relative rate method, Atkinson & Aschmann 1984)}

k_{NO_3} = 2.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \text{ (fast flow system/MS, Benter & Schindler 1988)}

k_{OH} = 6.66 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \text{ (recommended, Atkinson 1989)}

k_{NO_3} = (4.4 \pm 0.8) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 \pm 1 K} \text{ (FTIR, Andersson & Ljungström 1989)}

k_{OH} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{NO_3} = 7.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Atkinson 1990)}

k_{OH} = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \text{ (recommended, Atkinson 1991)}

k_{OH} = 6.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{NO_3} = 7.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (Sabljić & Gusten 1990)}

k_{OH} = 2.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{NO_3} = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{O(3P)} = 6.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \ k_{O(3P)} = 1.98 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for reaction with O(3P) atom at 298 K} \text{ (recommended, Atkinson 1997)}

Hydrolysis: will hydrolyze appreciably \text{ (Howard 1989)}.

Biodegradation: \ t_{1/2}^{(aerobic)} = 7 \text{ d}, \ t_{1/2}^{(anaerobic)} = 28 \text{ d} \text{ in natural waters} \text{ (Capel & Larson 1995)}

Biotransformation:

Half-Lives in the Environment:

Air: estimated photooxidation \ t_{1/2} = 0.24–24 \text{ h} \text{ (Darnall et al 1976)} \text{ for the reaction with hydroxyl radical; photooxidation with OH radicals with an estimated \ t_{1/2} \sim 3.1 \text{ h} \text{ (Lyman et al. 1982; quoted, Howard 1989); completely degraded within 6 h in a smog chamber irradiated by sunlight} \text{ (Kopcynski et al 1972; quoted, Howard 1989); \ t_{1/2} = 15 \text{ h} \text{ in air for the reaction with nitrate radical} \text{ (Atkinson et al. 1984a; quoted, Howard 1989); \ t_{1/2} = 0.76–7.8 \text{ h, based on measured photooxidation rate constants in air} \text{ (Howard et al. 1991). Surface water: \ t_{1/2} = 1200 to 48000 \text{ h, based on measured photooxidation rate constants with OH radicals in water} \text{ (Güsten et al. 1981; quoted, Howard et al. 1991); \ estimated \ t_{1/2} = 3.8 \text{ h for evaporation from a model river 1 m deep with a 1 m/s current and a 3 m/s wind} \text{ (Lyman et al. 1982; quoted, Howard 1989); \ t_{1/2} \sim 320 \text{ h and \ t_{1/2} = 9 \times 10^{4}} \text{ for oxidation by OH and RO}_2 \text{ radicals and \ t_{1/2} = 9 \times 10^{4} \text{ d for olefins in aquatic system, and \ t_{1/2} = 19 \text{ h, based on rate constant of 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1} \text{ for oxidation of dienes with singlet oxygen in aquatic system} \text{ (Mill & Mabey 1985); volatileizes rapidly with a half-life estimated to be several hours} \text{ (Howard 1989); \ t_{1/2} = 168–672 \text{ h, based on estimated aqueous aerobic biodegradation half-lives} \text{ (Howard et al. 1991) \ t_{1/2}^{(aerobic)} = 7 \text{ d, \ t_{1/2}^{(anaerobic)} = 28 \text{ d in natural waters} \text{ (Capel & Larson 1995). Ground water: \ t_{1/2} = 336–1344 \text{ h, based on estimated aqueous aerobic biodegradation half-lives} \text{ (Howard et al. 1991). Sediment: \ t_{1/2} = 168–672 \text{ h, based on estimated aqueous aerobic biodegradation half-lives} \text{ (Howard et al. 1991). Biota:}}

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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

\[
\log P = A - B/(T/K)
\]

(1)  \[
\ln P = A - B/(T/K)
\]

(1a)

\[
\log P = A - B/(C + t/°C)
\]

(2)  \[
\ln P = A - B/(C + t/°C)
\]

(2a)

\[
\log P = A - B/(T/K) - C\cdot\log(T/K)
\]

(3)

\[
\log P = A\cdot[1 - \Phi/(T/K)]
\]

(4)

where \(\log A = a + bT + cT^2\)

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<thead>
<tr>
<th>Heisig 1933</th>
<th>Stull 1947</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
<th>Flebbe et al. 1982</th>
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<td><strong>selected values</strong></td>
<td><strong>static-quartz manometer</strong></td>
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<td>-1.50</td>
<td>113857</td>
<td>-26.054</td>
<td>39997</td>
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| eq. 2 | P/mmHg | | |
| A | 6.84999 | | |
| B | 930.546 | | |
| C | 238.854 | | |

\(\Delta H_f/(kJ \text{ mol}^{-1})\) =

at 25°C 21.05

at bp 22.68

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FIGURE 2.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1,3-butadiene.
2.1.2.2.2 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: C₅H₈; CH₂=C(CH₃)CH=CH₂  
Molecular Weight: 68.118  
Melting Point (°C):  
−145.9 (Lide 2003)  
Boiling Point (°C):  
34 (Lide 2003)  
Density (g/cm³ at 20°C):  
0.6809, 0.6759 (20°C, 25°C, Dreisbach 1959)  
Molar Volume (cm³/mol):  
100.4 (20°C, calculated-density)  
103.6 (calculated-Le Bas method at normal boiling point)  
Enthalpy of Fusion, ΔHₘₜ (kJ/mol):  
4.92 (Chickos et al. 1999)  
Entropy of Fusion, ΔSₘₜ (J/mol K):  
38.68, 34.7 (exptl., calculated-group additivity method, Chickos et al. 1999)  
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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* (20°C, shake flask-GC, measured range 20–60°C, Pavlova et al. 1966)  
610* (recommended best value, IUPAC Solubility Data Series, temp range 20–60°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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):  
53329* (15.4°C, summary of literature data, temp range −79.8 to 32.6°C, Stull 1947)  
66816* (22.5°C, ebulliometry, measured range 16.8–34.8°C, Forziati et al. 1950)  
log (P/mmHg) = 6.90335 – 1080.996/(234.668 + t°C); temp range 16.8–34.8°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)  
3349* (−38.227°C, inclined-piston manometer, measured range −57.598 to −38.227°C, Osborn & Douslin 1969)  
73330 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)  
log (P/mmHg) = 6.90334 − 1080.996/(234.67 + t°C); temp range −35 to 84°C (Antoine eq. for liquid state, Dreisbach 1959)  
73300 (interpolated-Antoine eq., temp range −18.477 to 55.36°C, Zwolinski & Wilhoit 1971)  
73340* (derived from compiled data, Zwolinski & Wilhoit 1971)  
log (P/mmHg) = 6.88564 − 1071.578/(233.513 + t°C); temp range −18.477 to 55.36°C (Antoine eq., Zwolinski & Wilhoit 1971)  
73000, 78380 (calculated-Antoine eq., Boublík et al. 1984)  
log (P/kPa) = 6.05468 − 1095.41/(236.322 + t°C); temp range −58 to −38.2°C (Antoine eq. from reported expctl. data, Boublík et al. 1984)  
log (P/kPa) = 6.05329 − 1092.997/(236.002 + t°C); temp range −16 to 33°C (Antoine eq. from reported expctl. data, Boublík et al. 1984)
73350 (interpolated-Antoine eq., temp range –52 to –24°C, Dean 1985, 1992)

\[
\log (P/\text{mmHg}) = 7.01187 - 1126.159/(238.88 + t/°C); \text{ temp range –52 to –24°C (Antoine eq., Dean 1985, 1992)}
\]

\[
\log (P/\text{mmHg}) = 6.88564 - 1071.518/(233.51 + t/°C); \text{ temp range –19 to 55°C (Antoine eq., Dean 1985, 1992)}
\]

73350 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P_l/\text{kPa}) = 6.13677 - 1126.159/(-34.266 + T/K); \text{ temp range 221–254 K (Antoine eq.-I, Stephenson & Malanowski 1987)}
\]

\[
\log (P_l/\text{kPa}) = 6.0154 - 1071.578/(-39.637 + T/K); \text{ temp range 254–316 K (Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

73330, 10770 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

Henry’s Law Constant (Pa m³/mol at 25°C):

7840 (calculated-\(1/K_{AW}, C_w/C_A\), 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 \(K_{ow}\):

2.05 (calculated-regression eq. from Lyman et al. 1982, Wang et al. 1992)

1.91 (calculated-molar volume \(V_m\), Wang et al. 1992)

Octanol/Air Partition Coefficient, log \(K_{oa}\):

2.06 (calculated-measured \(\gamma^\infty\) in pure octanol and vapor pressure \(P\), Abraham et al. 2001)

Bioconcentration Factor, log \(BCF\):

Sorption Partition Coefficient, log \(K_{OC}\):

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

\[
k_{o3} = 16.5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 294 \pm 2 \text{ K (chemiluminescence, Adeniji et al. 1981)}
\]

\[
k_{o3}* = 1.25 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone in air at } 296 \text{ K, measured range } 278–323 \text{ K (static system-chemiluminescence, Atkinson et al. 1982)}
\]

\[
k_{oh}* = (9.26 \pm 1.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \text{ K, measured range } 299–422 \text{ K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982)}
\]

\[
k_{oh} = 10.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 297 \pm K, k_{oh}(calc) = 9.40 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (relative rate method, Ohta 1983)}
\]

\[
k_{o3}* = (0.58 – 1.25) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ between } 260–296 \text{ K (Atkinson & Carter 1984)}
\]

\[
k_{o3} = 1.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 0.8 \text{ d}^{-1}, k_{oh} = 9.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 8 \text{ d}^{-1}, \text{ and } k_{no3} = 5.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with a loss rate of } 12 \text{ d}^{-1} \text{ (Atkinson & Carter 1984)}
\]

\[
k_{no3} = (3.23 \pm 0.38) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \pm 1 \text{ K (relative rate method, Atkinson et al. 1984a)}
\]

\[
k_{no2} = (10.3 \pm 0.3) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with NO}_2 \text{ at } 295 \pm 2 \text{ K (relative rate method, Atkinson et al. 1984b)}
\]

\[
k_{o3} = 1.2 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{oh} = 9.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{no3} = 3.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson et al. 1984b)}
\]
k_{OH} = 10.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 295 \text{ K} \text{ (relative rate method, Atkinson & Aschmann 1984)}

k_{OH} = 9.98 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, 9.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 299 \text{ K} \text{ (Atkinson 1985)}

k_{OH} = (101 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 23.7 \pm 0.5 \text{ °C} \text{ (Edney et al. 1986)}

k_{NO_3} = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (Benter & Schindler 1988)}

k_{OH}^* = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (recommended, Atkinson 1989)}

k_{OH} = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{O_3} = 1.43 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (Atkinson 1990)}

k_{OH} = 5.91 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (Sabljic & Güsten 1990)}

k_{NO_3}^* = 6.78 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (recommended, Atkinson 1991)}

k_{OH}^* = 1.01 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3}^* = 6.78 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{O_3}^* = 12.8 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with } O(^3P) \text{ atom at } 298 \text{ K} \text{ (recommended, Atkinson 1997)}

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: calculated atmospheric lifetimes: 32 h due to reaction with O_3 in 24-h period, 2.9 h with OH radical during daytime, and 3.6 h for NO_3 radical during nighttime for “clean atmosphere”; 10 h for reaction with O_3 in 24-h period, 1.4 h with OH radical during daytime, and 22 min with 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 O_3, 2.9 h with OH radicals and 0.083 h with NO_3 radicals, all based on the reaction rate constants with O_3, OH and NO_3 radicals in the gas phase (Atkinson & Carter 1984)

Surface water: t_{1/2} \sim 320 h and 9 \times 10^4 d for oxidation by OH and RO_2 radicals for olefins in aquatic system, and t_{1/2} = 19 h, based on rate constant of 1.0 \times 10^7 M^{-1} 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

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<th>Shaw 1989a</th>
<th>Góral et al. 2004</th>
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<tr>
<td>20</td>
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FIGURE 2.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methyl-1,3-butadiene.

TABLE 2.1.2.2.2
Reported vapor pressures of 2-methyl-1,3-butadiene (isoprene) at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T} \quad (1)
\]

\[
\ln P = A - \frac{B}{T} \quad (1a)
\]

\[
\log P = A - \frac{B}{C + t/°C} \quad (2)
\]

\[
\ln P = A - \frac{B}{C + t/°C} \quad (2a)
\]

\[
\log P = A - \frac{B}{C + T/K} \quad (3)
\]

\[
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

\[
\log P = A[1 - \Phi/(T/K)] \quad (5) \text{ where } \log A = a + bT + cT^2
\]

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\( \Delta H_f / (\text{kJ mol}^{-1}) = \)\n\( \text{at } 25^\circ \text{C} \) | 26.44 |
\( \text{at bp} \) | 26.07 |
FIGURE 2.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-methyl-1,3-butadiene.

b.p. = 34 °C
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: C₆H₁₀; CH₂ = (CH₃)C(CH₃)=CH₂
Molecular Weight: 82.143
Melting Point (°C):
  –76 (Lide 2003)
Boiling Point (°C):
  68.8 (Lide 2003)
Density (g/cm³ at 20°C):
  0.7267, 0.7222 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
  113.0, 113.7 (20°C, 25°C, calculated-density)
  125.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₙₙ (kJ/mol):
Entropy of Fusion, ΔSₙₙ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  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°C and reported temperature dependence equations):
  19200 (calculated-Antoine eq., Dreisbach 1959)
log (P/mmHg) = 7.02388 – 1220.88/(225.9 + t°C); temp range –6 to 116°C (Antoine eq. for liquid state, Dreisbach 1959)
  20160 (interpolated-Antoine eq., Boublík et al. 1984)
log (P/kPa) = 6.25005 – 1302.766/(238.42 + t°C); temp range 0.04–68.6°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
  20160 (interpolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.1197 – 1299.69/(238.09 + t°C); temp range 0–68.5°C (Antoine eq., Dean 1985, 1992)
  20150 (interpolated-Stephenson & Malanowski 1987)
log (P/kPa) = 6.3266 – 1346.0/(–30.15 + T/K); temp range 273–342 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 29.9755 – 2.5677 × 10³/(T/K) – 7.8544·log (T/K) + 2.2361 × 10⁻¹⁰·(T/K)²; temp range 197–526 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
  4830 (calculated-1/Kₓₓₓ, Cₓ/Cₓ, reported as exptl., Hine & Mookerjee 1975)
  5420, 6990 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
  21100 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
Octanol/Water Partition Coefficient, log Kₒₜₜ:
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.25 \pm 0.05) \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 $\pm$ 2 K; $k_{OH}(\text{calc}) = 1.26 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (relative rate method, Ohta 1983)

$k_{OH} = 1.22 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 K (Atkinson 1985, 1989)

$k_{NO3} = 2.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Benter & Shindler 1988)

$k_{OH} = 1.22 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO3} = 1.052 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Sabljic & Güsten 1990)

$k_{NO3} = 2.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH} = 1.22 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO3} = 2.1 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{O3}^{*} = 26.5 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant $k = 1.0 \times 10^7$ M$^{-1}$ 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: C₅H₈; CH₂=CHCH₂CH=CH₂
Molecular Weight: 68.118
Melting Point (°C):
–148.2 (Lide 2003)
Boiling Point (°C):
26 (Lide 2003)
Density (g/cm³ at 20°C):
0.6608, 0.6557 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
103.1, 103.9 (20°C, 25°C, calculated-density)
103.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆H_fus (kJ/mol):
6.14 (Chickos et al. 1999)
Entropy of Fusion, ∆S_fus (J/mol K):
49.41, 52/3 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
558 (shake flask-GC, McAuliffe 1966)

Vapor Pressure (Pa at 25°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°C, Stull 1947)
63774* (20.669°C, ebulliometry, measured range 14.7–26.7°C (Forziati et al. 1950)
log (P/mmHg) = 6.84880 – 1025.016/(232.354 + t/°C); temp range 14.7–26.7°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
97900 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)
log (P/mmHg) = 6.84880 – 1025.016/(232.354 + t/°C); temp range –41 to 72°C (Antoine eq. for liquid state, Dreisbach 1959)
3611* (–43.083°C, inclined-piston manometer, measured range –60.01 to –43.083°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°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.83543 – 1017.995/(231.461 + t/°C); temp range –33.271 to 46.73°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 6826.6/(T/K)] + 7.899113; temp range –83.5 to 26.1°C (Antoine eq., Weast 1972–73)
98300, 99400 (extrapolated-Antoine equations, Boublik et al. 1984)
log (P/kPa) = 6.06018 – 1063.485/(236.447 + t/°C); temp range –78.84 to –18.08°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/kPa) = 6.34694 – 1239.949/(238.278 + t/°C); temp range –60.0 to –26.05°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
97930 (interpolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.17401 – 1155.378/(244.30 + t/°C); temp range –57 to –37°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.83543 – 1017.995/(231.461 + t/°C); temp range –33 to 47°C (Antoine eq., Dean 1985, 1992)
97900 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
Aliphatic and Cyclic Hydrocarbons

\[ \log (P_{L}/\text{kPa}) = 6.29891 - 1155.378/(–28.852 + T/K) \]; temp range 216–234 K (Antoine eq.-I, Stephenson & Malanowski 1987)

\[ \log (P_{L}/\text{kPa}) = 5.96033 - 1017.995/(–41.698 + T/K) \]; temp range 236–307 K (Antoine eq.-II, Stephenson & Malanowski 1987)

\[ \log (P/\text{mmHg}) = 23.7408 - 2.0505 \times 10^3/(T/K) - 5.679 \cdot \log (T/K) - 5.9671 \times 10^{-11} \cdot (T/K) + 1.1242 \times 10^{-6} \cdot (T/K)^2 \]; temp range 125–479 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m$^3$/mol at 25°C):

- 12140 (calculated/\$K_{AW}$, $C_W/C_A$, 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 $K_{OW}$:

- 2.48 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.48 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volutilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_O$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{OH} = (50.6 \pm 1.3) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 ± 2 K; $k_{OH}(\text{calc}) = 50.2 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (relative rate method, Ohta 1983)
- $k_{OH} = 5.33 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 K (Atkinson 1985, Atkinson 1989)
- $k_{OH} = 5.1 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp (Atkinson et al. 1984b)
- $k_{NO3} = 7.8 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (fast flow system, Benter & Shindler 1988)
- $k_{OH} = 5.3 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant $k = 1.0 \times 10^7$ M$^{-1}$ 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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{(T/K) - C \log (T/K)} \quad (4) \\
\log P &= A \left[1 + \frac{\Phi}{T/K}\right] \quad (5) \text{ where } \log A = a + b T + c T^2
\end{align*}
\]

Stull 1947

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<th>t/°C</th>
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Forziati et al. 1950

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Osborn & Douslin 1969

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Zwolinski & Wilhoit 1971

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Summary of literature data

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Antoine eq.

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Cox eq.

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eq. 5

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ΔHf/(kJ mol⁻¹) =

| at 25°C | 25.15 |
| at bp | 25.15 |
FIGURE 2.1.2.4.1 Logarithm of vapor pressure versus reciprocal temperature for 1,4-pentadiene.
### 1,5-Hexadiene

**Common Name:** 1,5-Hexadiene  
**Synonym:**  
**Chemical Name:** 1,5-Hexadiene  
**CAS Registry No:** 592-42-7  
**Molecular Formula:** C\textsubscript{6}H\textsubscript{10}; CH\textsubscript{2}=CH(CH\textsubscript{2})\textsubscript{2}CH=CH\textsubscript{2}  
**Molecular Weight:** 82.143  
**Melting Point (°C):**  
–140.7 (Lide 2003)  
**Boiling Point (°C):**  
59.4 (Lide 2003)  
**Density (g/cm\textsuperscript{3} at 20°C):**  
0.6920 (Weast 1984)  
0.6923, 0.6878 (20°C, 25°C, Dreisbach 1959)  
**Molar Volume (cm\textsuperscript{3}/mol):**  
119.0 (20°C, calculated-density, Wang et al. 1992)  
125.8 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):**  
**Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):**  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):**  
169 (shake flask-GC, McAuliffe 1966)  
320 (14°C, calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)  
**Vapor Pressure (Pa at 25°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)  
\[ \log (P/\text{mmHg}) = 7.00740 - 1184.99/(227.7 + t/°C); \text{temp range -13 to 102°C (Antoine eq. for liquid state, Dreisbach 1959)} \]  
32077* (26.95°C, static method-Hg manometer, measured range 26.95–46.13°C, Letcher & Marsicano 1974)  
29690 (interpolated-Antoine eq., Dean 1985, 1992)  
\[ \log (P/\text{mmHg}) = 6.5741 - 1013.5/(214.8 + t/°C); \text{temp range 0–59°C (Antoine eq., Dean 1985, 1992)} \]  
29670, 29690 (interpolated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)  
\[ \log (P_i/kPa) = 5.7368 - 1032.0/(-56.15 + T/K); \text{temp range 273–333 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]  
\[ \log (P_i/kPa) = 5.98314 - 1159.908/(-40.998 + T/K); \text{temp range 299–333 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]  
\[ \log (P/\text{mmHg}) = 10.5886 - 2.0106 \times 10^3/(T/K) + 0.28813 \log (T/K) - 9.562 \times 10^{-3}(T/K) + 7.164 \times 10^{-6}(T/K)^2; \text{temp range 132–507 K (vapor pressure eq., Yaws 1994)} \]  
**Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):**  
13620 (calculated-1/K\textsubscript{AW} C\textsubscript{w}/C\textsubscript{A}, reported as exptr., 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 \(K_{\text{ow}}\):**  
2.40 (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)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH} = 6.16 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 ± 2 K (relative rate method, Ohta 1983)

$k_{OH} = 6.35 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $5.85 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with 1,3-butadiene and propylene as standard substances respectively at 297 ± 2 K (relative rate method, Ohta 1983)

$k_{OH} = 6.2 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_{1/2} = 19$ h, based on rate constant of $1.0 \times 10^7$ M$^{-1}$ s$^{-1}$ for oxidation of dienes by singlet oxygen in aquatic system (Mill & Mabey 1985).

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**TABLE 2.1.2.2.5.1**

Reported vapor pressures of 1,5-hexadiene at various temperatures

<table>
<thead>
<tr>
<th>Letcher &amp; Marsicano 1974</th>
</tr>
</thead>
<tbody>
<tr>
<td>static method-Hg manometer</td>
</tr>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>26.95</td>
</tr>
<tr>
<td>28.93</td>
</tr>
<tr>
<td>31.62</td>
</tr>
<tr>
<td>34.54</td>
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<tr>
<td>36.94</td>
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<tr>
<td>39.96</td>
</tr>
<tr>
<td>41.77</td>
</tr>
<tr>
<td>43.04</td>
</tr>
<tr>
<td>46.13</td>
</tr>
</tbody>
</table>

Antoine eq.:

$log P = A - B/(C + T/K)$

| P/mmHg |
| A | 6.6228 |
| B | 1037.35 |
| C | -55.52 |
FIGURE 2.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 1,5-hexadiene.
2.1.2.2.6 1,6-Heptadiene

Common Name: 1,6-Heptadiene
Synonym:
Chemical Name: 1,6-heptadiene
CAS Registry No: 3070-53-9
Molecular Formula: C_7H_12
Molecular Weight: 96.170
Melting Point (°C):
   −129 (Lide 2003)
Boiling Point (°C):
   90 (Lide 2003)
Density (g/cm³ at 20°C): 0.714
Molar Volume (cm³/mol):
   134.0 (20°C, calculated-density, McAuliffe 1966; Wang et al. 1992)
   148.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
   44.0 (shake flask-GC, McAuliffe 1966)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
   2.90 (calculated-π substituent constants, Hansch et al. 1968)
   2.73 (calculated-MCI χ, Murray et al. 1975)
   3.31 (calculated-fragment const., Müller & Klein 1992)
   2.85 (calculated-molar volume V_{M}, Wang et al. 1992)
   3.2189 (calculated-UNIFAC group contribution, Chen et al. 1993)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constant and Half-Lives:
Halflives in the Environment:
   Surface water: t_{1/2} ~ 320 h and 9 × 10⁴ d for oxidation by OH and RO₂ radicals for olefins in aquatic system, and
t_{1/2} = 19 h, based on rate constant of 1.0 × 10⁷ M⁻¹ 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: C₄H₆, CH₃CH₂C≡CH
Molecular Weight: 54.091
Melting Point (°C):
-125.7 (Lide 2003)
Boiling Point (°C):
8.08 (Lide 2003)
Density (g/cm³ at 20°C):
0.650. 0.65 (20°C, 25°C, at saturation pressure, Dreisbach 1959)
Molar Volume (cm³/mol):
83.22 (20°C, calculated-density)
81.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hfusion (kJ/mol):
6.03 (Chickos et al. 1999)
Entropy of Fusion, ∆Sfusion (J/mol K):
40.9, 36.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
2870 (shake flask-GC, at 1 atmospheric pressure, McAuliffe 1966)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
log (P/mmHg) = 6.97497 – 986.46/(232.85 + t°C); temp range –67 to 43°C (Antoine eq. for liquid state, Dreisbach 1959)
188251 (derived from compiled data, Zwolsinski & Wilhoit 1971)
log (P/mmHg) = 7.07338 – 1101.71/(235.81 + t°C); temp range –30.8 to 26.8°C (Antoine eq., Zwolsinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 6596.9/(T/K)] + 8.032581; temp range –92.5 to 8.7°C (Antoine eq., Weast 1972–73)
log (P/mmHg) = 6.98198 – 988.75/(233.01 + t°C); temp range –68 to 27°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.98198 – 988.75/(233.01 + t°C); temp range 147–443 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
1880 (calculated-1/KAW, CW/C_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 χ, Nirmalakhandan & Speece 1988)
1846 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log KOW:
1.44, 1.48 (quoted, calculated-molar volume V_M, Wang et al. 1992)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{O3} = 1.79 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (static system-IR, Dillemuth et al. 1963)

$k_{O3} = (33 \pm 5) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 $\pm$ 1 K (static system-UV, DeMore 1971)

$k_{O3} = (19.7 \pm 2.6) \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 $\pm$ 2 K (relative rate method, Atkinson et al. 1984b)

$k_{OH} = (10.42 \pm 1.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987)

$k_{OH} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{O3} = 2.0 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{O3} = 1.79 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K; and $1.79 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $4.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (literature review, Atkinson 1991)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
2.1.2.3.2 1-Pentyne

Common Name: 1-Pentyne
Synonym: pent-1-yne
Chemical Name: 1-pentyne
CAS Registry No: 627-19-0
Molecular Formula: C₅H₈; CH≡C(CH₂)₂CH₃
Molecular Weight: 68.118
Melting Point (°C):
  –90 (Lide 2003)
Boiling Point (°C):
  40.1 (Lide 2003)
Density (g/cm³ at 20°C):
  0.6901, 0.6849 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
  98.71, 99.46 (20°C, 25°C, calculated-density)
  103.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH₉₀ (kJ/mol):
Entropy of Fusion, ΔS₉₀ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  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°C and reported temperature dependence equations):
  57520 (calculated from determined data, Dreisbach 1959)
  \[
  \log \left( \frac{P}{\text{mmHg}} \right) = 6.97263 - 1095.42/(227.53 + t/°C); \text{ temp range } -50 \text{ to } 70°C \text{ (Antoine eq. for liquid state, Dreisbach 1959)}
  \]
  57600 (interpolated-Antoine eq., temp range –33 to 61°C Zwolinski & Wilhoit 1971)
  57462 (derived from compiled data, Zwolinski & Wilhoit 1971)
  \[
  \log \left( \frac{P}{\text{mmHg}} \right) = 7.04614 - 1092.52/(227.18 + t/°C); \text{ temp range } -33 \text{ to } 61°C \text{ (Antoine eq., Zwolinski & Wilhoit 1971)}
  \]
  57540 (interpolated-Antoine eq., temp range –44 to 61°C, Dean 1985)
  \[
  \log \left( \frac{P}{\text{mmHg}} \right) = 6.96734 - 1092.52/(227.18 + t/°C); \text{ temp range } -44 \text{ to } 61°C \text{ (Antoine eq.}, \text{ Dean 1985, 1992)}
  \]
  57540 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
  \[
  \log \left( \frac{P}{\text{mmHg}} \right) = 6.09224 - 1092.52/(-45.97 + T/K); \text{ temp range } 229–315 \text{ K (Antoine eq., Stephenson & Malanowski 1987)}
  \]
  \[
  \log \left( \frac{P}{\text{mmHg}} \right) = 33.8369 - 2.4684 \times 10^{13}(T/K) - 9.4301\log (T/K) + 6.1345 \times 10^{-10}(T/K) + 4.676 \times 10^{-6}(T/K)^2;
  \text{ temp range } 167–481 \text{ K (vapor pressure eq., Yaws 1994)}
  \]
Henry’s Law Constant (Pa m²/mol at 25°C):
  2536 (calculated-1/Kₐₘₜ, Cₙ/Cₙ, 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 χ, Nirmalakhandan & Speece 1988)
  4983 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log Kₐₘₜ:
  1.98 (shake flask-UV, Hansch et al. 1968, Hansch & Anderson 1967)
  2.12 (generator column-GC, Tewari et al. 1982a,b)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatileization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_{O3}$ with O3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = (11.17 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987, quoted, Atkinson 1989)

$k_{NO3} = 7.54 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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: C₆H₁₀; C₄H₉C≡CH
Molecular Weight: 82.143
Melting Point (°C):
–131.9 (Dreisbach 1959; Lide 2003)
Boiling Point (°C):
71.33 (Dreisbach 1959)
71.3 (Lide 2003)
Density (g/cm³ at 20°C):
0.7155, 0.7155 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
114.8 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
125.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₚ (kJ/mol):
Entropy of Fusion, ΔSₘₚ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°C):
18140 (calculated-Antoine eq., Dreisbach 1959)
\[ \log (P/\text{mmHg}) = 6.91212 - 1194.6/(225.0 + t/°C); \text{ temp range } -8 \text{ to } 118°C \] (Antoine eq. for liquid state, Dreisbach 1959)
18145 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/\text{kPa}) = 6.03702 - 1194.6/(-48.15 + T/K); \text{ temp range } 265–391 K \] (Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/\text{mmHg}) = 55.7231 - 3.2541 \times 10^3/(T/K) - 18.405 \log (T/K) + 9.5814 \times 10^{-3}(T/K) + 9.2278 \times 10^{-14}(T/K)^2; \text{ temp range } 141–516 K \] (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol):
4020 (calculated-1/Kₘₕ, Cₖ/Cₘ, reported as exptl., Hine & Mookerjee 1975)
4210, 4020 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
4310 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
2166 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log Kₖₙₜ:
2.48 (calculated-π 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 $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}^* = (12.6 \pm 0.04) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 253–343 K (discharge flow-resonance fluorescence, Boodaghians et al. 1987; quoted, Atkinson 1989)

$k_{NO3} = 1.60 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (Atkinson 1991)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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: C\(_7\)H\(_{12}\)
Molecular Weight: 96.170
Melting Point (°C):
-81  (Lide 2003)
Boiling Point (°C):
99.7  (Lide 2003)
Density (g/cm\(^3\) at 20°C):
0.7330  (Weast 1984)
0.7328, 0.7283  (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm\(^3\)/mol):
131.2  (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
148.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):

Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°C):
94.0  (shake flask-GC, McAuliffe 1966)
107  (calculated-recommended liquid-liquid equilibrium LLE data, Góral et al. 2004)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
7000  (Antoine eq., Dreisbach 1959)
4298  (extrapolated-Antoine eq., Boublík et al. 1984)
\[ \log (P/\text{Pa}) = 6.27249 - 1314.492/(208.097 + t/°C); \text{ temp range 63.1–99.98°C} \] (Antoine eq. from reported exptl. data, Boublík et al. 1984)
7500  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/\text{kPa}) = 6.4039 - 1392.4/(-56.55 + T/K); \text{ temp range 336–373 K} \] (Antoine eq., Stephenson & Malanowski 1987)
\[ \log (P/\text{mmHg}) = 38.1255 - 3.064 \times 10^3/(T/K) - 10.679 \log (T/K) + 3.668 \times 10^{-6} \times (T/K)^2; \text{ temp range 154–537 K} \] (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m\(^3\)/mol at 25°C):
6830  (calculated-1/K\(_{\text{AW}}\), C\(_{\text{aw}}\)/C\(_{\text{A}}\), reported as exptl., Hine & Mookerjee 1975)
5950, 6090  (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
5420  (calculated-MCI \(\chi\), Nirmalakhandan & Speeke 1988)
7160  (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):
2.98  (calculated-\(\pi\) substituent constants, Hansch et al. 1968)
2.93  (calculated-MCI \(\chi\), Murray et al. 1975)
2.98  (calculated-molar volume \(V_M\), 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 $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

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: C₈H₁₄; C₆H₁₃C≡CH
Molecular Weight: 110.197
Melting Point (°C):
-79.3 (Dreisbach 1959; Lide 2003)
Boiling Point (°C): 127–128
126.3 (Lide 2003)
Density (g/cm³ at 20°C):
0.7461, 0.7419 (20°C, 25°C, Dreisbach 1959)
Molar Volume (cm³/mol):
147.7 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
170.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₙₑₑ (kJ/mol):
Entropy of Fusion, ΔSₙₑₑ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equations):
1813 (calculated-Antoine eq., Dreisbach 1959)
log (P/μmHg) = 7.02447 – 1413.8/(215.0 + t°C); temp range 25–170°C (Antoine eq. for liquid state, Dreisbach 1959)
1723 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.36895 – 1997.558/(202.608 + t°C); temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1715 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.19321 – 1427.434/(–214.625 + T/K); temp range 84.8–126.26 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol at 25°C):
8208 (calculated-1/Kₘₜₜ, Cₘ/Cₜ, reported as exptl., Hine & Mookerjee 1975)
8208, 9000 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
6827 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
8325 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log Kₐₖₜ:
3.48 (calculated-π substituent constants, Hansch et al. 1968)
3.37 (calculated-MCI χ, Murray et al. 1975)
3.49 (calculated-molar volume Vₘₜ, 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, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{f}$:

Half-Lives in the Environment:
### 1-Nonyne

**Common Name:** 1-Nonyne  
**Synonym:**  
**Chemical Name:** 1-nonyne  
**CAS Registry No:** 3452-09-3  
**Molecular Formula:** C₉H₁₆; C₇H₁₅C≡CH  
**Molecular Weight:** 124.223  
**Melting Point (°C):**  
-50 (Dreisbach 1959; Lide 2003)  
**Boiling Point (°C):** 150–151  
150.8 (Dreisbach 1959; Lide 2003)  
**Density (g/cm³ at 20°C):**  
0.7570 (Weast 1984)  
0.7568, 0.7527 (20°C, 25°C, Dreisbach 1959)  
**Molar Volume (cm³/mol):**  
164.1 (20°C, calculated-density, McAuliffe 1966; Ruelle & Kesselring 1997)  
192.4 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, ΔHₚₜₚ (kJ/mol):**  
**Entropy of Fusion, ΔSₚₜₚ (J/mol K):**  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m³ or mg/L at 25°C):**  
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°C):**  
835 (calculated-Antoine eq., Dreisbach 1959; quoted, Hine & Mookerjee 1975)  
log (P/mmHg) = 6.77410 – 1404.7/(210.0 + t°C); temp range 50–223°C (Antoine eq. for liquid state, Dreisbach 1959)  
**Henry’s Law Constant (Pa m³/mol):**  
14600 (calculated-1/Kₐₘₑ, Cₙ/Cₘ, reported as exptl., Hine & Mookerjee 1975)  
11600, 13010 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)  
8700 (calculated-MCI χ, Nirmalakhandan & Speece 1988)  
14400 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)  
**Octanol/Water Partition Coefficient, log K₀ₐₘₑ:**  
3.98 (calculated-π substituent constants, Hansch et al. 1968)  
3.81 (calculated-MCI χ, Murray et al. 1975)  
3.98 (calculated-molar volume Vₚₚ, 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 K₀ₐ:**  
**Bioconcentration Factor, log BCF:**  
**Sorption Partition Coefficient, log Kₒₑ:**  
**Environmental Fate Rate Constants, k, and Half-Lives, tᵢₑ:**  
**Half-Lives in the Environment:**

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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: C₅H₈
Molecular Weight: 68.118
Melting Point (°C): –135.0 (Lide 2003)
Boiling Point (°C): 44.2 (Lide 2003)
Density (g/cm³ at 20°C):
0.7720, 0.7665 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol):
88.2 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
92.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
27.92, 26.96 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔHfus (kJ/mol):
0.48, 3.36; 3.84 (~–186.08, –135.05°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔSfus (J/mol K):
29.83, 37.6 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section.):
39890* (19.77°C, static method-quartz spiral gauge, measured range –42.75 to 19.77°C, Lister 1941)
43375* (21.028°C, ebulliometry, measured range 11.3–45.024°C, Forziati et al. 1950)
log (P/mmHg) = 6.92066 – 1121.818/(233.446 + t/°C); temp range 11.3–45.0°C (Antoine eq., ebulliometry, Forziati et al. 1950)
50690 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 6.92066 – 1121.818/(233.446 + t/°C); temp range –30 to 105°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/atm) = [1– 317.520/(T/K)] × 10^8{0.814441 – 7.42372 × 10⁻⁴(T/K) + 8.49035 × 10⁻³(T/K)^²}; temp range: 223.2–393.2 K (Cox eq., Chao et al. 1983)
log (P/mmHg) = 6.92066 – 1121.818/(223.45 + t/°C); temp range not specified (Antoine eq., Dean 1985, 1992)
50710 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 30.1132 – 2.3537 × 10⁻³(T/K) – 8.0609× 10⁻¹(T/K)²; temp range 138–507 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

6370 (calculated-1/Kₐₑₐₑ, Cₓ/w/Cₐₓ, 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)


Octanol/Water Partition Coefficient, log _K_ₐₒₕₐₜ:
1.75 (calculated-π substituent const., Hansch et al. 1968)
1.76 (calculated-molar volume _V_m_, Wang et al. 1992)
2.25 (calculated-fragment const., Muller & 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 _K_ₐₒₐ:

Bioconcentration Factor, log _B_ₐₙ₇:

Sorption Partition Coefficient, log _K_ₐₙₜ:

Environmental Fate Rate Constants, _k_, and Half-Lives, _t_ₕₐₜ:

Volutilization:

Photolysis:

Oxidation: rate constant _k_, for gas-phase second order rate constants, _k_₁ for reaction with OH radical, _k_ₐₙ₇ for reaction with _O_₅ radical and _k_ₐₕ₃ with _O_₃ as indicated, *data at other temperatures see reference:

_k_₁₃ = 8.13 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 298 K (Japar et al. 1974; quoted, Adeniji et al. 1981)

_k_ₐ₉₃ = 9.69 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (chemiluminescence, Adeniji et al. 1981)

_k_₁₉₃ = (2.75 ± 0.33) × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 297 ± 1 K (Atkinson et al. 1983a)

_k_₂ₕ₉ = (6.39 ± 0.23) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 ± 2 K (relative rate method, Atkinson et al. 1983b)

_k_₁₉₃ = 4.97 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ at 291.5 K in synthetic air (Bennett et al. 1987)

_k_₂ₕ₉ = (62.4 ± 3.5) × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ at 297 ± 2 K in a smog chamber (Nolting et al. 1988)

_k_₃ₙ₉ = 4.99 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 ± 3 K, and _k_₃ₙ₉ = 5.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ relative to propene (relative rate method, Rogers 1989)

_k_₃ₜ₉ = (5.02 – 6.73) × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K (literature review, Atkinson 1989)

_k_₄ₜ₉ = 4 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at 298 K, _k_₅₉₉ = 4.6 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (Atkinson 1990)

_k_₆₉₉ = 6.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, _k_₅₉₉ = 5.81 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ at 298 K (Sablje & Güsten 1990)

_k_₆ₙ₉ = 6.7 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹, _k_₅ₙ₉ = 5.3 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹, _k_₆ₗ₉ = 5.7 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹, and _k_₅ₗ₉ = 2.1 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with O(P) atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (_k_₃₉) and Elimination (_k_₃₉) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photooxidation rate constant of 4.97 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹ for the reaction with _O_₅ in synthetic air was determined at atmospheric pressure at 291.5 K (Bennett et al. 1987); rate constant _k_ = 4.99 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ for the reaction with OH radicals in air at 298 K (Rogers 1989).

Surface water: _t_ₕ = 320 h and 9 × 10⁴ d for oxidation by OH and RO₂ radicals in aquatic system, and _t_ₕ = 40 d, based on rate constant _k_ = 2 × 10⁶ M⁻¹ 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) + D \cdot [P/(T/K)^2] \quad (5) \\
\log \left( \frac{P}{\text{atm}} \right) &= A' \left[ 1 - \left( \frac{T_B}{T} \right) \right] \quad (6)
\end{align*}
\]

where \( \log A' = a + bT + cT^2 \)

<table>
<thead>
<tr>
<th>Lister 1941</th>
<th>Forziati et al. 1950</th>
<th>Bakierowska &amp; Trzeszczyński 2003</th>
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<tr>
<td></td>
<td></td>
<td>B</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
</tr>
</tbody>
</table>

\( \ln (1/K_{aw}) = 6.989 - 1915/(T/K) \)

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: C₆H₁₀
Molecular Weight: 82.143

Melting Point (°C):
-103.5 (Weast 1982–83; Lide 2003)

Boiling Point (°C):
82.98 (Lide 2003)

Density (g/cm³ at 20°C):
0.8110, 0.8061 (20°C, 25°C, Dreisbach 1959)
0.8102 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
101.4 (calculated-density, Stephenson & Malanowski 1987; Ruelle & Kesselring 1997)
110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆HV (kJ/mol):
33.142, 30.485 (25°C, bp, Riddick et al. 1986)

Enthalpy of Vaporization, ∆HV (kJ/mol):
29.125, 27.276 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ∆Hfus (kJ/mol):
3.28 (Riddick et al. 1986)
4.23, 3.28; 7.51 (−134.45, −104.45°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, ΔSfus (J/mol K):
49.85, 41.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Pierotti & Liabastre 1972)
281, 286 (23.5°C, 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°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* (−44.42, −24.85, 0. 18.45°C, static method-quartz spiral gauge, Lister 1941)
11734* (24.794°C, ebulliometry, measured range 12.2–83.9°C (Forziati et al. 1950)
log (P/mmHg) = 6.888617 − 1229.973/(224.104 + t°C); temp range 12.2–83.9°C (Antoine eq., ebulliometry measurements, Forziati et al. 1950)
11840 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 6.88617 − 1229.73/(224.104 + t°C); temp range 3.0–146°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/mmHg) = [1− 356.172/(T/K)] × 10^8[0.873674 − 9.73841 × 10^{-4}·(T/K) + 10.9078 × 10^{-7}·(T/K)^2]; temp range 213.2–364.53 K (Cox eq., Chao et al. 1983)
Aliphatic and Cyclic Hydrocarbons

\[ \log(P/kPa) = 7.109 - 2289.0/(T/K); \] temp range: not specified (Antoine eq., Riddick et al. 1986)

\[ \log(P/kPa) = 5.997323 - 1221.899/(–49.978 + T/K); \] temp range 309–385 K (Antoine eq., Stephenson & Malanowski 1987)

\[ \log(P/mmHg) = 52.1749 - 3.238 \times 10^3/(T/K) - 16.878 \times 10^{-3} \times(T/K) + 1.3259 \times 10^{-13} \times(T/K)^2; \] temp range 170–560 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated):

\[ 4020 \] (calculated-1/K AW, CW/CA, 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)

\[ 3960 \] (23°C, batch air stripping-IR, Nielsen et al. 1994)


Octanol/Water Partition Coefficient, log \(K_{OW}\):

\[ 2.16 \] (calculated-π 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 \(K_{OA}\) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

\[ 2.92^* \] (20.29°C, from GC-determined γ∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)

\[ 2.83 \] (calculated-measured γ∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log \(BCF\):

Sorption Partition Coefficient, log \(K_{OC}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_1/2\):

Volatilization:

Photolysis:

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{OH}\) for reaction with OH radical, \(k_{NO3}\) with NO₃ radical and \(k_{O3}\) with O₃ or as indicated, *data at other temperatures see reference:

\[ k_{O3P} = 2.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction with O(3P) atom (Herron & Huie 1973)} \]

\[ k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (relative rate method, Atkinson et al. 1979)} \]

\[ k_{O3} = 1.69 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (Japar et al. 1974)} \]

\[ k_{O3} = 2.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 294 ± 2 K (chemiluminescence, Adeniji et al. 1981)} \]

\[ k_{O3} = (1.04 \pm 0.14) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 297 ± 1 K (Atkinson et al. 1983a)} \]

\[ k_{OH} = (6.43 \pm 0.17) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 ± 2 K (relative rate method, Atkinson et al. 1983b)} \]

\[ k_{OH} = (64.1 \pm 2.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 297 ± 2 K (relative rate method, Ohta 1983)} \]

\[ k_{O3} = 1.04 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 297 K (Atkinson & Carter 1984)} \]

\[ k_{O3} = 1.04 \times 10^{-16} \text{ cm}^3 \text{ molecul} e^{-1} \text{ s}^{-1} \text{ with O(3P) atom and } k_{NO3} < 0.2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ with NO}_3 \text{ (Atkinson & Aschmann 1984)} \]

\[ k_{O3} = 1.51 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ in synthetic air at 295 K (Bennett et al. 1987)} \]

\[ k_{O3} = (7.8 \pm 0.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 297 ± 2 K in a smog chamber (Nolting et al. 1988)} \]

\[ k_{OH} = 5.40 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K and } k_{OH} = 6.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ relative to propene (relative rate method, Rogers 1989)} \]

\[ k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1989)} \]

\[ k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} , \text{ } k_{NO3} = 5.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (Atkinson 1990)} \]

\[ k_{OH} = 6.75 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} , \text{ } k_{NO3} = 5.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (Sabljic & Güsten 1990)} \]
$k_{NO_3} = 5.28 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (quoted, Atkinson 1991)

$k_{OH} = 6.77 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3^*} = 5.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{O_3^*} = 8.14 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O(3P)$ atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Surface water: $t_{1/2} \sim 320 \text{ h}$ and $9 \times 10^4 \text{ d}$ for oxidation by OH and RO$_2$ radicals in aquatic system, and $t_{1/2} = 40 \text{ d}$ based on rate constant $k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ 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

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<th>Temperature</th>
<th>Solubility</th>
<th>Temperature</th>
<th>Solubility</th>
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<td>S/g·m$^{-3}$</td>
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<tr>
<td>5.11</td>
<td>280</td>
<td>5</td>
<td>–</td>
<td>5.1</td>
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<td>15.21</td>
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<td>15</td>
<td>–</td>
<td>15.2</td>
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<td>299</td>
<td>20</td>
<td>–</td>
<td>20</td>
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<td>302.5</td>
<td>25</td>
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**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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\ln P &= A - B/(T/K) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(C + T/K) - C \cdot \log (T/K) \\
\log (P/\text{atm}) &= A'\left[1 - \left(\frac{T_B}{T}\right)\right] \\
\end{align*}
\]

where \( A' = a + bT + cT^2 \)

<table>
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<tr>
<th>Vapor pressure</th>
<th>log ( K_{OA} )</th>
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<tbody>
<tr>
<td>static-quartz spiral gauge</td>
<td>ebulliometry</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( P/\text{Pa} )</td>
</tr>
<tr>
<td>(-44.42)</td>
<td>160</td>
</tr>
<tr>
<td>(-24.85)</td>
<td>752</td>
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<tr>
<td>0</td>
<td>3345</td>
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<tr>
<td>18.45</td>
<td>8723</td>
</tr>
<tr>
<td>( \Delta H_v/(\text{kJ mol}^{-1}) = 32.59 ) at 27°C</td>
<td>( \text{bp/°C} )</td>
</tr>
<tr>
<td>63.200</td>
<td>53712</td>
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<tr>
<td>69.708</td>
<td>66808</td>
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<td>76.766</td>
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<td>81.757</td>
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<td>82.791</td>
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<td>83.353</td>
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<td>83.852</td>
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<td>eq. 2</td>
<td>( \text{P/mmHg} )</td>
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<tr>
<td>A</td>
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<td>B</td>
<td>1229.973</td>
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<tr>
<td>C</td>
<td>224.104</td>
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<td>( \text{bp/°C} )</td>
<td>82.979</td>
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</table>
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 $K_{OA}$ 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: C₇H₁₂
Molecular Weight: 96.170
Melting Point (°C):
−120.4 (Lide 2003)
Boiling Point (°C):
110.3 (Lide 2003)
Density (g/cm³ at 20°C):
0.8102, 0.8058 (20°C, 25°C, Dreisbach 1959; Weast 1982–83)
Molar Volume (cm³/mol):
118.7 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
133.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
37.75, 32.70 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH₉ᵤ (kJ/mol):
6.63 (Chickos et al. 1999)
Entropy of Fusion, ΔS₉ᵤ (J/mol K):
43.16, 44.1 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C: F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°C or as indicated and reported temperature dependence equations):
4080 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 6.86861 − 1308.0/(218.0 + t°C); temp range 25–165°C, (Antoine eq. for liquid state, Dreisbach 1955)
3933 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P₁/kPa) = 6.0101 − 1311.087/(-56.045 + T/K); temp range 333–384 K (Antoine eq., Stephenson & Malanowski 1987)
4858 (25.25°C, transpiration method, Verevkin et al. 2000)
ln (P/P₀) = 23.65 – 4531/(T/K); temp range 275.4–313.4 K (transpiration method, Verevkin et al. 2000)
Henry’s Law Constant (Pa m³/mol at 25°C):
7660 (calculated-1/Kₘ₆, Cₚ/Cₜ, reported as exptl., Hine & Mookerjee 1975)
7485, 14260(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
11070 (calculated-MCI χ, Nirmalakhandan & Speece 1988)
Octanol/Water Partition Coefficient, log Kₙₚₙ:
1.05 (calculated-regression of Lyman et al. 1982, Wang et al. 1992)
2.20 (calculated-molar volume Vₘ, Wang et al. 1992)
Octanol/Air Partition Coefficient, log Kₙ₉ₐ:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures see reference:

$k_{OH} = 9.44 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 305 K (Darnall et al. 1976, Atkinson 1989)

$k_{NO3} = (2.87 \pm 0.34) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (relative rate method, Atkinson et al. 1984a)

$k_{O3} < 0.20 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH} = 6.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{NO3} = 2.9 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; and $k_{O(3P)} = 2.1 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with O(3P) atom at room temp. (relative rate method, Atkinson et al. 1984b)

$k_{OH} = 9.45 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 294 K (Atkinson 1985)

$k_{OH} = 9.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{OH} = 9.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO3} = 1.7 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{O3} = 1.65 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{O(3P)} = 9.0 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction with O(3P) atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_{1/2} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals in aquatic system, and $t_{1/2} = 40$ d, based on rate constant $k = 2 \times 10^8$ M$^{-1}$ 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: C\textsubscript{7}H\textsubscript{12}
Molecular Weight: 96.170
Melting Point (°C):
–56 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
115 (Weast 1982–83; Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.8228 (Weast 1982–83)
Molar Volume (cm\textsuperscript{3}/mol):
116.9 (20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
129.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
36.73 (27°C, Lister 1941)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
5.28, 0.71, 0.97; 6.96 (–119.15, –63.15, –56.15°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
42.14, 45.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
66.0 (shake flask-GC, McAuliffe 1966)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
188, 821, 2636, 6547 (–21.44, 0, 19.82, 39.06°C, static method-quartz spiral gauge, Lister 1941)
2670 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P\textsubscript{v}/kPa) = 7.27243 – 2011.9/(T/K); temp range 251–313 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol):
Octanol/Water Partition Coefficient, log K\textsubscript{ow}:
2.57 (calculated-π 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 $V_M$, Wang et al. 1992)
3.37 (calculated-fragment const., Müller & Klein 1992)
Octanol/Air Partition Coefficient, log K\textsubscript{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K\textsubscript{oc}:
Environmental Fate Rate Constants, k, and Half-Lives, $t_\text{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k\textsubscript{OH} for reaction with OH radical, k\textsubscript{NO3} with NO\textsubscript{3} radical and k\textsubscript{O3} with O\textsubscript{3} or as indicated, *data at other temperatures see reference:
\( k_{O_3} = (3.19 \pm 0.36) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 297 ± 1 K (Atkinson et al. 1983a; quoted, Atkinson & Carter 1984)

\( k_{OH} = (7.08 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (relative rate method, Atkinson et al. 1983b)

\( k_{OH} = 7.44 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Atkinson et al. 1983b, Atkinson 1989)

\( k_{O_3} = (28.3 \pm 1.5) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 297 ± 2 K in a smog chamber (Nolting et al. 1988)

\( k_{NO_3} = 2.80 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH} = 7.13 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Sabljic & Güsten 1990)

\( k_{NO_3} = 4.84 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (Atkinson 1991)

\( k_{OH} = 7.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 4.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \) and \( k_{O_3}^* = 2.45 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: \( t_{1/2} \sim 320 \text{ h and } 9 \times 10^4 \text{ d for oxidation by OH and RO}_2 \text{ radicals in aquatic system, and } t_{1/2} = 40 \text{ d, based on rate constant } k = 2 \times 10^5 \text{ M}^{-1} \text{ s}^{-1} \) for oxidation of cyclic olefins by singlet oxygen in aquatic system (Mill & Mabey 1985).
2.1.2.4.5 Cyclooctene

Common Name: Cyclooctene
Synonym:
Chemical Name: cyclooctene
CAS Registry No: 931-87-3 (cis-octene), 931-89-5 (trans-octene)
Molecular Formula: C₈H₁₄
Molecular Weight: 110.197
Melting Point (°C):
-12, -59 (cis-, trans-cyclooctene, Weast 1982–83; Lide 2003)
-14.5 to -15.5 (cis-cyclooctene, Stephenson & Malanowski 1987)
Boiling Point (°C):
Density (g/cm³):
0.8472, 0.8483 (20°C, cis-, trans-cyclooctene, Weast 1982–83)
Molar Volume (cm³/mol):
130.1 (cis-, 20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
129.9 (trans-, 20°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, ΔHᵥ (kJ/mol):
41.57 (27°C, Lister 1941)
Enthalpy of Sublimation, ΔHₛₜₜ (kJ/mol):
Entropy of Fusion, ΔSᵋₜ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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/τ + 43.2804·ln τ, τ = [(T/K)/298.15], temp range 273.15–313.15 K (generator column-GC/FID, Dohányosová et al. 2004)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
209.3, 774.6, 2333, 5948 (0, 19.83, 40.36, 60.22°C, static method-quartz spiral manometer, Lister 1941)
log (Pₑ/KPa) = 7.3641 – 2194.3/(T/K), temp range 273–441 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 (Pa m³/mol at 25°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 Kₑₒₜₜ:
Octanol/Air Partition Coefficient, log Kₒₐ:
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log Kₒₑ:
Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:

Volatilization:
Photolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3}
with NO_3 radical and k_{O3} with O_3 or as indicated, *data at other temperatures see reference:
k_{O3}^* = 3.75 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} (\text{cis}-\text{cyclooctene}, \text{ recommended, Atkinson 1997})

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

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<th>TABLE 2.1.2.4.5.1</th>
<th>Reorted aqueous solubilities and Henry's law constants of cyclooctene at various temperatures</th>
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<tbody>
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<td>Aqueous solubility</td>
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<td>Dohányosová et al. 2004</td>
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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 1,4-Cyclohexadiene

Common Name: 1,4-Cyclohexadiene
Synonym: 1,4-dihydrobenzene
Chemical Name: 1,4-cyclohexadiene
CAS Registry No: 628-41-1
Molecular Formula: C₆H₈
Molecular Weight: 80.128
Melting Point (°C): -49.2 (Weast 1983–83; Lide 2003)
Boiling Point (°C): 85.5 (Lide 2003)
Density (g/cm³ at 20°C): 0.8471 (Weast 1982–83)
Molar Volume (cm³/mol):
93.60 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
103.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₕus (kJ/mol): 0.82, 5.72; 6.53 (–81.15, –49.15°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔSₕus (J/mol K):
29.16, 38.0 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Pierotti & Liabstre 1972)
800* (recommended, temp range 5–45°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°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°C, static method-Hg manometer, measured range 304.25–322.23 K, Letcher & Marsicano 1974)
log (P/mmHg) = [1– 368.566/(T/K)] × 10^4[0.916704 – 6.81678 × 10⁻⁴·(T/K) – 7.02362 × 10⁻⁷·(T/K)²]; temp range 304.25–322.23 K (Cox eq., Chao et al. 1983)
8973 (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.86553 – 1176.707/(214.528 + t°C); temp range 31.1–49.08°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
9009 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.41736 – 1475.149/(–26.108 + T/K); temp range: 304–360 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log Kₐw:
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 Kₐa:
Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\text{½}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO3}}$ with NO$_3$ radical and $k_{\text{O3}}$ with O$_3$ or as indicated, *data at other temperatures see reference:

- $k_{\text{O3}} = (0.639 \pm 0.074) \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 297 ± 1 K (Atkinson et al. 1983a)
- $k_{\text{OH}} = (9.48 \pm 0.39) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 2 K (relative rate method, Atkinson et al. 1983b)
- $k_{\text{NO3}} = (2.89 \pm 0.035) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (Atkinson et al. 1984a)
- $k_{\text{O3}} = 63.9 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{\text{OH}} = 9.5 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{\text{NO3}} = 0.29 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{\text{NO2}} < 0.4 \times 10^{-20}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with NO$_2$ (Atkinson et al. 1984b)
- $k_{\text{OH}}(\text{exptl}) = 9.90 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{\text{OH}}(\text{calc}) = 1.03 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson 1985)
- $k_{\text{NO3}} = 7.8 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (fast flow system, Benter & Schindler 1988)
- $k_{\text{OH}} = (99.2 – 99.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (review, Atkinson 1989)
- $k_{\text{OH}} = 9.91 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{\text{NO3}} = 5.30 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction with NO$_3$ radical at nights (Sabljic & Güsten 1990)
- $k_{\text{NO3}} = 6.6 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1991)
- $k_{\text{OH}} = 9.95 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{\text{NO3}} = 6.6 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{\text{NO3}} = 4.6 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: $t_\text{½} \sim 320$ h and $9 \times 10^4$ d for oxidation by OH and RO$_2$ radicals for olefins in aquatic system, and $t_\text{½} = 19$ h, based on rate constant $k = 1.0 \times 10^7$ M$^{-1}$ 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

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<td>S/g·m$^{-3}$</td>
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<td>900</td>
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<td>1000</td>
<td>25.1</td>
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<td>1000</td>
<td>35.2</td>
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</tr>
</tbody>
</table>

**Antoine eq., P/mmHg**

$log P = A – B/(C + T/K)$

- **A** = 7.2687
- **B** = 1461.75
- **C** = 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 Cycloheptatriene

Common Name: Cycloheptatriene
Synonym: tropilidene
Chemical Name: 1,3,5-cycloheptatriene
CAS Registry No: 544-25-2
Molecular Formula: C7H8
Molecular Weight: 92.139
Melting Point (°C):
–79.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
117 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
0.8875 (Weast 1982–83)
Molar Volume (cm³/mol):
103.0 (20°C, calculated-density, McAuliffe 1966; Lande & Banerjee 1981; Wang et al. 1992)
114.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₚᵤₛ (kJ/mol):
2.35, 1.16; 3.51 (–93.15, –75.15°C, Chickos et al. 1999)
Entropy of Fusion, ΔSₚᵤₛ (J/mol K):
21.11, 38.5 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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* (25.11°C, shake flask-GC, measured range 5.11–40.21°C, Pierotti & Liabastre 1972)
640* (recommended best value, temp range 5–45°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°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°C, Finke et al. 1956)
log (P/mmHg) = 6.97032 – 1374.065/(t/°C + 220.538); temp range 0–65°C (Antoine eq., ebulliometry, Finke et al. 1956)
2825, 3138 (interpolated-Antoine eq-I, II, Stephenson & Malanowski 1987)
log (P/kPa) = 6.09522 – 1374.656/(–52.612 + T/K); temp range 273–390 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 6.12574 – 1390.771/(–53.069 + T/K); temp range 273–390 K (Antoine eq.-II, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol at 25°C):
432 (calculated-P/C from selected data)
466 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log Kₐω:
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 $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{OH} = (5.39 \pm 0.078) \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{O3} = (9.12 \pm 0.23) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for at 294 ± 2 K (Atkinson et al. 1984b)

$k_{OH} = 5.39 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for at 294 K (Atkinson & Carter 1984)

$k_{NO3} = 1.18 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{OH} = 9.44 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Sabljic & Güsten 1990)

$k_{OH} = 96.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 294 K (Atkinson 1989)

$k_{NO3} = 1.19 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (quoted, Atkinson 1991)

$k_{OH} = 9.7 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO3} = 1.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{O3} = 5.4 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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

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<th>Aqueous solubility</th>
<th>Vapor pressure</th>
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<td>Pierotti &amp; Liabastre 1972</td>
<td>Finke et al. 1956</td>
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<td>Shaw 1989a</td>
<td>IUPAC recommended</td>
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<tr>
<td>shake flask-GC</td>
<td>IUPAC recommended</td>
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### TABLE 2.1.2.4.7.1 (Continued)

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<th>Source</th>
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<th>Vapor pressure</th>
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<td>Pierotti &amp; Liabastre 1972</td>
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<tr>
<td>shake flask-GC</td>
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<td>t/°C</td>
<td>S/g·m⁻³</td>
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<tr>
<td>445</td>
<td>0.0031</td>
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<tr>
<td>∆HV/(kJ mol⁻¹) = 38.70</td>
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<tr>
<td>at 25°C</td>
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</tbody>
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- **Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclohepta-triene.**

- **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  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: C₁₀H₁₆
Molecular Weight: 136.234
Melting Point (°C):
−74  (Lide 2003)
Boiling Point (°C):
178  (Weast 1982–83; Lide 2003)
Density (g/cm³ at 25°C):
0.8403, 0.8383 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
162.1  (20°C, calculated-density, Stephenson & Malanowski 1987)
192.2  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
45.1  (25°C, Riddick et al. 1986)
Enthalpy of Fusion, ΔHₕₚ (kJ/mol):
Entropy of Fusion, ΔSₕₚ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°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 (P/mmHg) = [−0.2185 × 10508.4/(T/K)] + 8.016262; temp range 14.0–175°C (Antoine eq., Weast 1972–73)
2670  (68.2°C, Riddick et al. 1986)
278, 202  (calculated-Antoine eq.-I, II, Stephenson & Malanowski 1987)
log (P₁/kPa) = 6.81591 − 2075.62/(–16.65 + T/K); temp range 287–448 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P₂/kPa) = 7.67098 – 2494.342/(T/K); temp range 288–323 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 9.3771 – 2.8246 × 10³/(T/K) + 1.0584·log (T/K) – 8.9107 × 10⁻³·(T/K)²; temp range 199–660 K (vapor pressure eq., Yaws 1994)
213  (activity coefficient-GC, Fichan et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°C):
2725  (calculated-P/C from selected data)
Octanol/Water Partition Coefficient, log Kₒₜₜₜ:
4.38  (RP-HPLC-RT correlation, Griffin et al. 1999)
Octanol/Air Partition Coefficient, log Kₒₐₜₜ:

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Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K<sub>OC</sub>:

Environmental Fate Rate Constants, k, and Half-Lives, t<sub>½</sub>:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k<sub>OH</sub> for reaction with OH radical, k<sub>NO3</sub> with NO<sub>3</sub> radical and k<sub>O3</sub> with O<sub>3</sub> or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

- k<sub>OH</sub> = 9 × 10<sup>10</sup> cm<sup>3</sup> mol<sup>−1</sup> s<sup>−1</sup>, with t<sub>OH</sub> < 0.24 h (Darnall et al. 1976)
- k<sub>OH</sub> = (9.0 ± 1.35) × 10<sup>10</sup> M<sup>−1</sup> s<sup>−1</sup> at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)
- k<sub>OH</sub> = 9.0 × 10<sup>10</sup> M<sup>−1</sup> s<sup>−1</sup>, k<sub>O3</sub> = 3.9 × 10<sup>8</sup> M<sup>−1</sup> s<sup>−1</sup>, and k<sub>OH(O3P)</sub> = (6.50 ± 0.52) × 10<sup>10</sup> cm<sup>3</sup> M<sup>−1</sup> s<sup>−1</sup> for reaction with O<sup>(3P)</sup> atom at room temp. (Winer et al. 1976)
- k<sub>OH(calc)</sub> = 13.8 × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup>, k<sub>OH(obs.)</sub> = (14.0, 14.2) × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> (Atkinson et al. 1983b)
- k<sub>NO3</sub> = (7.7 ± 1.7) × 10<sup>−12</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> at 295 K (relative rate technique, Atkinson et al. 1984a)
- k<sub>O3</sub> = 6.4 × 10<sup>−16</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with calculated lifetimes τ = 6 min and 11 min in 24-h in clean and moderately polluted atmosphere, respectively; k<sub>OH</sub> = 1.42 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with calculated τ = 2.0 h and 1.0 h during daytime in clean and moderately polluted atmosphere respectively, k<sub>NO3</sub> = 7.7 × 10<sup>−12</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with calculated τ = 9 min and 0.9 min during nighttime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)
- k<sub>NO2</sub> < 3.5 × 10<sup>−20</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> for gas phase reaction with NO<sub>2</sub> at 295 K (Atkinson et al. 1984b)
- k<sub>O3</sub> = 6.4 × 10<sup>−16</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup>; k<sub>OH</sub> = 1.42 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup>, k<sub>NO3</sub> = 7.7 × 10<sup>−12</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> and k<sub>OH(O3P)</sub> = 1.29 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with O<sup>(3P)</sup> atom at room temp. (Atkinson et al. 1984b)
- k<sub>O3</sub> = 6.0 × 10<sup>−16</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with a loss rate of 36 d<sup>−1</sup>; k<sub>OH</sub> = 1.4 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with a loss rate of 12 d<sup>−1</sup>, and k<sub>NO3</sub> = 1.4 × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with a loss rate of 290 d<sup>−1</sup> (Atkinson & Carter 1984)
- k<sub>O3</sub> = 6.0 × 10<sup>−16</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with a loss rate of 36 d<sup>−1</sup>; k<sub>OH</sub> = 1.7 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with a loss rate of 7.3 d<sup>−1</sup>, and k<sub>NO3</sub> = 1.4 × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with a loss rate of 290 d<sup>−1</sup> at room temp. (Atkinson 1985)
- k<sub>OH</sub> = (16.9 ± 0.5) × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> at 294 ± 1 K (relative rate method, Atkinson et al.1986)
- k<sub>OH</sub> = 6.4 × 10<sup>−16</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with calculated τ = 36 min; k<sub>OH</sub> = 1.7 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with τ(calc) = 1.6 h, k<sub>NO3</sub> = 1.4 × 10<sup>−12</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> with τ(calc) = 5.0 min for clean tropospheric conditions at room temp. (Atkinson et al. 1986)
- k<sub>OH</sub> = (146–171) × 10<sup>−12</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> at 294–305 K (review, Atkinson 1989)
- k<sub>OH</sub> = 1.71 × 10<sup>−10</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup>, k<sub>NO3</sub> = 1.22 × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup>, k<sub>O3</sub> = 2.03 × 10<sup>−16</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> and k<sub>OH(O3P)</sub> = 7.2 × 10<sup>−11</sup> cm<sup>3</sup> molecule<sup>−1</sup> s<sup>−1</sup> for the reaction with O<sup>(3P)</sup> atom, at 298 K (recommended, Atkinson 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k<sub>1</sub>) and Elimination (k<sub>2</sub>) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: t<sub>OH</sub> < 24 h in air based on its photooxidation rate constant of 9 × 10<sup>13</sup> cm<sup>3</sup> mol<sup>−1</sup> s<sup>−1</sup> for the gas phase reaction with hydroxyl radical (Darnall et al. 1976; Lloyd et al. 1976); calculated lifetimes: τ = 36 min due to reaction with O<sub>3</sub> in 24-h period, τ = 2.0 h with OH radical during daytime, and τ = 9 min for NO<sub>3</sub> radical during nighttime for “clean” atmosphere; τ = 11 min for reaction with O<sub>3</sub> in 24-h period, τ = 1.0 h with OH radical during daytime, and τ = 0.9 min for NO<sub>3</sub> radical during nighttime in moderately polluted atmosphere (Atkinson et al. 1984a); calculated atmospheric lifetimes, τ = 36 min, 1.6 h and 5.0 min for reaction with O<sub>3</sub>, OH and NO<sub>3</sub> radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986); calculated tropospheric lifetimes τ = 1.1 h, 1.9 h and 53 min due to reactions with OH radical, O<sub>3</sub> and NO<sub>3</sub> radical, respectively, at room temp. (Corchnoy & Atkinson 1990).
2.1.2.4.9 \(\alpha\)-Pinene

Common Name: \(\alpha\)-Pinene
Synonym: \(dl\)-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: \(\text{C}_{10}\text{H}_{16}\)
Molecular Weight: 136.234
Melting Point (°C):
-55 (\(dl\)-Form, Weast 1982–83)
-64 (\(d\)-Form, Riddick et al. 1986; Lide 2003)
-50 (\(d\)-Form, Stephenson & Malanowski 1987)
Boiling Point (°C):
156.2 (\(dl\)-Form, Weast 1982–83; Lide 2003)
156 (\(d\)-Form, Stephenson & Malanowski 1987)
155–156 (\(d\)-, \(l\)-Form, Budavari 1989)
Density (g/cm\(^3\)):
0.8582 (20°C, \(dl\)-Form, Weast 1982–83)
0.8582, 0.8539 (\(d\)-Form, Riddick et al. 1986)
0.8592, 0.8591, 0.8590 (20°C, \(dl\)-, \(d\)-, \(l\)-Form, Budavari 1989)
Molar Volume (cm\(^3\)/mol):
157.4 (\(d\)-Form, Stephenson & Malanowski 1987)
183.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
46.61, 39.673 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C, \(F\): 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
21.8, 3.42; 5.04 (quoted lit. values; shake flask-GC/FID, Fichan et al. 1999)
Vapor Pressure (Pa at 25°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 (22.2, 22.5°C, measured range 21.1–148°C, Pickett & Peterson 1929)
237.3* (13.25°C, Hg manometer, measured range –6.0 to 13.25°C, Linder 1931)
666.6* (24.6°C, summary of literature data, temp range –1.0 to 155.0°C, Stull 1947)
678 (interpolated-Antoine eq., Weast 1972–73)
\[\log (P/\text{mmHg}) = [–0.2185 \times 9813.6/(T/K)] + 7.898207; \text{ temp range –1.0 to 155°C (Antoine eq., Weast 1972–73)}\]
667 (Verschueren 1983)
605, 587 (interpolated-Antoine equations, Boublik et al. 1984)
\[\log (P/\text{Pa}) = 6.37971 – 1692.803/(231.558 + t/°C); \text{ temp range 21.1–148°C (Antoine eq. from reported exptl. data of Pickett & Peterson 1929, Boublik et al. 1984)}\]
\[\log (P/\text{Pa}) = 6.95174 – 1430.936/(206.42 + t/°C); \text{ temp range 19.44–155.75°C (Antoine eq. from reported exptl. data of Hawkins & Armstrong 1954, Boublik et al. 1984)}\]
655 (selected, Riddick et al. 1986)
\[\log (P/\text{Pa}) = 25.52644 – 3134.525/(T/K) – 6.16045\log (T/K) (\text{Riddick et al. 1986})\]
Henry’s Law Constant (Pa m³/mol at 25°C or indicated. Additional data at other temperatures designated * are compiled at the end of this section.):

0.194* (20°C, calculated from measured liquid-phase diffusion coefficients, measured range −10 to 20°C, Zhang et al. 2003)

\[ \ln \left[ \frac{H'}{M\text{atm}} \right] = -6.590 + \frac{3800}{(T/K)} \]; temp range 263–293 K (Zhang et al. 2003)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

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 \( K_{OA} \);

Bioconcentration Factor, log \( BCF \) or log \( K_B \);

Sorption Partition Coefficient, log \( K_{OC} \);

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants \( k_{O3} \) for reaction with \( O_3 \), \( k_{OH} \) with \( OH \) radical and \( k_{NO3} \) with \( NO_3 \) radical at 25°C or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[ k_{OH} = (3.48 \pm 0.52) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1} \] at 305 ± 2 K (relative rate method, Winer et al. 1976)

\[ k_{OH} = 3.5 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}, k_{O3} = 2.0 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}, \] and \( k_{O3(3P)} = (1.60 \pm 0.06) \times 10^{10} \text{ M}^{-1} \text{ s}^{-1} \) for reaction with \( O(3P) \) atom at room temp. (Winer et al. 1976)

\[ k_{OH} = 32 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{O3} = 67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at room temp. (Gaffney & Levine 1979)

\[ k_{O3} = (8.4 \pm 1.9) \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 296 K, measured range 276–324 K, atmospheric lifetime \( \tau = 3–4 \) h due to reaction with \( O_3 \), and \( \tau \sim 4 \) h due to reaction with OH radical (Atkinson et al. 1982)

\[ k_{OH} = (6.01 \pm 0.82) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K, measured range 298–422 K (flash photolysis–resonance fluorescence, Kleindienst et al. 1982)

\[ k_{OH(calc)} = 8.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH(obs)} = (7.6, 5.5, 6.01) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] (Atkinson et al. 1983b)

\[ k_{OH}^{*} = 60.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K, measured range 298–422K (Flash photolysis–resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)

\[ k_{O3} = (3.4 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 295 ± 1 K (relative rate method, Atkinson et al. 1984a)

\[ k_{O3} = 8.4 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with calculated lifetimes of 4.6 h and 1.4 h in 24-h in clean and moderately polluted atmosphere, respectively; \( k_{O3} = 6.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) with calculated lifetimes of 4.6 h and 2.3 h during daytime in clean and moderately polluted atmosphere, respectively, \( k_{NO3} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) 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)

\[ k_{NO2} < 2.1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] for gas phase reaction with \( NO_2 \) at 295 K (Atkinson et al. 1984b)
Aliphatic and Cyclic Hydrocarbons

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:
Air: calculated lifetimes: $\tau = 4.6$ h due to reaction with $O_3$ in 24-h period, $\tau = 4.6$ h with OH radical during daytime, and $\tau = 20$ min for NO$_3$ radical during nighttime for clean atmosphere; $\tau = 1.4$ h for reaction with $O_3$ in 24-h period, $\tau = 2.3$ h with OH radical during daytime, and $\tau = 2$ min with NO$_3$ radical during nighttime in moderately polluted atmosphere (Atkinson et al. 1984a, Winer et al. 1984); calculated atmospheric lifetimes of 5.6 h, 5.1 h and 11 min for reaction with $O_3$, OH and NO$_3$ radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986); calculated tropospheric lifetimes of 3.4 h, 4.6 h and 2.0 h due to reactions with OH radical, $O_3$ and NO$_3$ radicals 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

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>$t/°C$</th>
<th>P/Pa</th>
<th>$t/°C$</th>
<th>P/Pa</th>
</tr>
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<tr>
<td>21.2</td>
<td>533</td>
<td>134.9</td>
<td>57128</td>
<td>-6.0</td>
<td>54.66</td>
<td>-1.0</td>
<td>133</td>
</tr>
<tr>
<td>22.0</td>
<td>573</td>
<td>135.4</td>
<td>57608</td>
<td>1.0</td>
<td>96.0</td>
<td>24.6</td>
<td>666.6</td>
</tr>
<tr>
<td>22.2</td>
<td>640</td>
<td>138.5</td>
<td>63728</td>
<td>13.25</td>
<td>237.3</td>
<td>37.3</td>
<td>1333</td>
</tr>
<tr>
<td>22.5</td>
<td>800</td>
<td>138.8</td>
<td>64261</td>
<td>51.4</td>
<td>2666</td>
<td>51.4</td>
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(Continued)
### TABLE 2.1.2.4.9.1 (Continued)

<table>
<thead>
<tr>
<th>Pickett &amp; Peterson 1929</th>
<th>Linder 1931</th>
<th>Stull 1947</th>
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<tbody>
<tr>
<td>Ramsay &amp; Young method</td>
<td>Hg manometer</td>
<td>summary of literature data</td>
</tr>
<tr>
<td>*t/°C  P/Pa  *t/°C  P/Pa</td>
<td>*t/°C  P/Pa</td>
<td>*t/°C  P/Pa</td>
</tr>
<tr>
<td>54.7  3040  139.8  65861</td>
<td>66.8  5333</td>
<td></td>
</tr>
<tr>
<td>55.3  3200  140.1  66794</td>
<td>76.8  7999</td>
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</tr>
<tr>
<td>55.5  3306  140.5  67461</td>
<td>90.1  13332</td>
<td></td>
</tr>
<tr>
<td>77.4  7839  141.2  68794</td>
<td>110.2  26664</td>
<td></td>
</tr>
<tr>
<td>77.5  7906  141.3  69327</td>
<td>132.3  53329</td>
<td></td>
</tr>
<tr>
<td>77.7  7959  141.9  70394</td>
<td>155.0  101325</td>
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<tr>
<td>77.9  8026  147.0  80526</td>
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<td>79.3  8519</td>
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<td>mp/°C  –55</td>
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<td>103.8  21451</td>
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<td>132.9  54275</td>
<td></td>
<td></td>
</tr>
<tr>
<td>133.0  54755</td>
<td></td>
<td></td>
</tr>
<tr>
<td>133.1  54862</td>
<td></td>
<td></td>
</tr>
<tr>
<td>133.2  54995</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.

### Hawkins & Armstrong 1954

<table>
<thead>
<tr>
<th>Hg manometer</th>
</tr>
</thead>
<tbody>
<tr>
<td>*t/°C  P/Pa  *t/°C  P/Pa</td>
</tr>
<tr>
<td>------------</td>
</tr>
<tr>
<td>19.45  408.0  65.63  4858</td>
</tr>
<tr>
<td>21.3  457.3  66.54  5121</td>
</tr>
<tr>
<td>27.25  654.6  68.27  5554</td>
</tr>
<tr>
<td>29.72  790.6  70.45  6073</td>
</tr>
<tr>
<td>37.07  1201  75.1  7430</td>
</tr>
<tr>
<td>46.92  2015  76.04  7698</td>
</tr>
<tr>
<td>53.69  2832  77.12  8033</td>
</tr>
<tr>
<td>54.18  2877  79.75  8905</td>
</tr>
<tr>
<td>56.57  3234  84.71  10859</td>
</tr>
<tr>
<td>57.09  3309  86.23  11536</td>
</tr>
<tr>
<td>57.3  3393  88.42  12512</td>
</tr>
<tr>
<td>62.28  4221  92.01  14299</td>
</tr>
</tbody>
</table>
FIGURE 2.1.2.4.9.1 Logarithm of vapor pressure versus reciprocal temperature for α-pinene.

TABLE 2.1.2.4.9.2
Reported Henry's law constants of α-pinene at various temperatures

Zhang et al. 2003

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>–10</td>
<td>0.0397</td>
</tr>
<tr>
<td>0</td>
<td>0.0618</td>
</tr>
<tr>
<td>10</td>
<td>0.113</td>
</tr>
<tr>
<td>20</td>
<td>0.194</td>
</tr>
</tbody>
</table>

\[
\ln (k_H/\text{atm}) = A - \frac{B}{T/\text{K}}
\]
eq 3

H'/(M atm⁻¹)

A

–6.59

B

3800
FIGURE 2.1.2.4.9.2  Logarithm of Henry’s law constant versus reciprocal temperature for α-pinene.
2.1.2.4.10  β-Pinene

Common Name: β-Pinene
Synonym: β-Pinene d, or nopinene; β-Pinene l, or 2(10)-pinene
Chemical Name: 6,6-dimethyl-2-methylene bicyclo[3.1.1]heptane
CAS Registry No: 19172-67-3
Molecular Formula: C_{10}H_{16}
Molecular Weight: 136.234

Melting Point (°C):
-61.54 (l-Form, Riddick et al. 1986)
-50 (l-Form, Stephenson & Malanowski 1987)
-61.5 (l-Form, Lide 2003)

Boiling Point (°C):
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)

Density (g/cm³):
0.8654, 0.8694 (20°C, d-, l-Form, Weast 1982–83)
0.8667 (25°C, l-Form, Riddick et al. 1986)

Molar Volume (cm³/mol):
157.4 (l-Form, Stephenson & Malanowski 1987)
183.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):
43.471, 40.208 (25°C, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
32.7, 6.27; 11.04 (quoted lit. values; shake flask-GC, Fichan et al. 1999)

Vapor Pressure (Pa at 25°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°C, Pickett & Peterson 1929)
666.6* (30.0°C, summary of literature data, temp range 4.2–158.3°C, Stull 1947)
501 (interpolated-Antoine eq., Weast 1972–73)
log (P/mmHg) = [–0.2185 × 10235.8/(T/K)] + 8.633424; temp range 4.2–158.3°C (Antoine eq., Weast 1972–73)
667 (Verschueren 1983)
395 (interpolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.02052 – 1509.944/(210.05 + t°C); temp range 18.71–165.9°C (Antoine eq. from reported exptl. data of Hawkins & Armstrong 1954, Boublik et al. 1984)
610 (selected, Riddick et al. 1986)
log (P/kPa) = 27.90258 – 3318.845/(T/K) – 6.94263·log (T/K) (Riddick et al. 1986)
391 (l-Form, interpolated-Antoine eq., temp range 291–441K, Stephenson & Malanowski 1987)
log (P/kPa) = 6.04993 – 1520.15/(T/K + 62.75); temp range 291–441 K (l-Form, Antoine eq., liquid, Stephenson & Malanowski 1987)
log (P/mmHg) = 6.8984 – 1511.7/(t/°C + 210.2); temp range 19–156°C (Antoine eq., Dean 1992)

log (P/mmHg) = 7.067997 –1539.348/(T/K) –59.937; temp range 364–439 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)

log (P/mmHg) = 46.3728 – 3.9789 × 103/(T/K) –13.284·log (T/K) – 1.3113 × 10–10·(T/K)2; temp range 120–651 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m3/mol):

Octanol/Water Partition Coefficient, log K_{OW}:
4.16 (RP-HPLC-RT correlation, Griffin et al. 1999)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF or log K_{b}:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatile: rate constant k, for second order gas-phase rate constants k_{OH}, k_{O3} and k_{NO3} for reactions with OH radicals, O_3 and NO_3 radicals or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH} = 42 × 10^9 L mol^{-1} s^{-1}, with t_{1/2} = 0.24–2.4 h (Darnall et al. 1976)

k_{OH} = (4.06 ± 0.61) × 10^{10} M^{-1} s^{-1} at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

k_{OH} = 4.1 × 10^{10} M^{-1} s^{-1}; k_{O3} = 2.2 × 10^{11} M^{-1} s^{-1}; and k_{O_{3P}} = (1.51 ± 0.06) × 10^{10} M^{-1} s^{-1} for reaction with O(3P) atom (Winer et al. 1976)

k_{O3} = 30 × 10^{-12} cm^3 molecule^{-1} s^{-1}; k_{OH} = 65 × 10^{-12} cm^3 molecule^{-1} s^{-1} at room temp. (Gaffney & Levine 1979)

k_{OH} = (2.1 ± 0.5) × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K with atmospheric lifetime τ ~ 13 h due to reaction with O_3 and τ ~ 4 h due to reaction with OH radical (Atkinson et al. 1982)

k_{OH} = (7.76 ± 1.1) × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K, measured range 297–423 K (flash photolysis-resonance fluorescence, Kleindienst et al. 1982; Atkinson 1985)

k_{OH} = 5.1 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{OH}^{obs} = (6.4, 7.76) × 10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson et al. 1983b)

k_{NO3} = (1.4 ± 0.3) × 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 ± 1 K (relative rate method, Atkinson et al. 1984a)

k_{O3} = 2.1 × 10^{-17} cm^3 molecule^{-1} s^{-1} with calculated lifetimes τ = 18 h and 5.5 h in 24-h in clean and moderately polluted atmosphere respectively; k_{OH} = 7.8 × 10^{-11} cm^3 molecule^{-1} s^{-1} with calculated τ = 3.6 h and 1.8 h during daytime in clean and moderately polluted atmosphere, respectively; k_{NO3} = 1.4 × 10^{-12} cm^3 molecule^{-1} s^{-1} with calculated τ = 50 min and 5 min during nighttime in clean and moderately polluted atmosphere, respectively, at room temp. (Atkinson et al. 1984a)

k_{NO2} = < 2.4 × 10^{-20} cm^3 molecule^{-1} s^{-1} for gas phase reaction with NO_2 at 295 K (Atkinson et al. 1984b)

k_{O3} = 2.1 × 10^{-17} cm^3 molecule^{-1} s^{-1}; k_{OH} = 7.8 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 1.4 × 10^{-12} cm^3 molecule^{-1} s^{-1}; and k_{O_{3P}} = 640 × 10^{-18} cm^3 molecule^{-1} s^{-1} for the reaction with O(3P) atom, at room temp. (Atkinson et al. 1984b)

k_{OH} = (7.95 ± 0.52) × 10^{-11} cm^3 molecule^{-1} s^{-1} with calculated τ = 18 h; k_{OH} = 8.0 × 10^{-11} cm^3 molecule^{-1} s^{-1} with calculated τ = 3.5 h, k_{NO3} = 2.5 × 10^{-12} cm^3 molecule^{-1} s^{-1} with τ(calc) = 28 min for clean tropospheric conditions at room temp. (Atkinson et al. 1986)

k_{O3} = 2.36 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 ± 2 K (relative rate method, Atkinson et al. 1988)

k_{O3} = (1.4 ± 0.2) × 10^{-17} cm^3 molecule^{-1} s^{-1} at 297 ± 2 K in a smog chamber (Nolting et al. 1988)

k_{OH} = 7.89 × 10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (recommended, Atkinson 1989)

k_{OH} = 7.89 × 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{NO3} = 2.36 × 10^{-12} cm^3 molecule^{-1} s^{-1}, and k_{O3} = (2.1; 1.4) × 10^{-17} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson et al. 1990)
k_{OH} = 5.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{NO_3} = 2.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \quad \text{(Müller & Klein 1991)}

k_{OH} = 7.82 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ at 298K (Sabljić & Güsten 1990)}

k_{NO_3} = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (recommended, Atkinson 1991)}

k_{OH} = 7.82 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ at 298K (Sabljic & Güsten 1990)}

k_{NO_3} = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 22 \pm 1°C (Grosjean et al. 1993)}

k_{OH}^* = 7.89 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{NO_3} = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ and k}_{O_3}^* = 1.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \text{ for the reaction with O}\(^{(3P)}\) \text{ atom, at 298 K (recommended, Atkinson 1997)}

k_{OH, \text{lit}} = 7.95 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; k_{OH,\text{calc}} = 6.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (quoted; calculated-QSAR, Peters et al. 1999)}

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: calculated lifetimes: \( \tau = 18 \text{ h} \) due to reaction with O_3 in 24-h period, \( \tau = 3.6 \text{ h} \) with OH radical during daytime, and \( \tau = 50 \text{ min} \) for NO_3 radical during nighttime for “clean” atmosphere; \( \tau = 5.5 \text{ h} \) for reaction with O_3 in 24-h period, \( \tau = 1.8 \text{ h} \) with OH radical during daytime, and \( \tau = 5 \text{ min} \) with NO_3 radical during nighttime hours in “moderately polluted” atmosphere (Atkinson et al.1984a, Winer et al. 1984); calculated atmospheric lifetimes of 18 h, 3.5 h and 28 min for reaction with O_3, OH and NO_3 radicals respectively for clean tropospheric conditions at room temp. (Atkinson et al. 1986); calculated tropospheric lifetimes of 2.3 h, 1.1 d and 4.9 h due to reactions with OH radical, O_3 and NO_3 radical respectively at room temp. (Corchnoy & Atkinson 1990).

### TABLE 2.1.2.4.10.1

Reported vapor pressures of β-pinene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

\[
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \quad (3)
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TABLE 2.1.2.4.10.1 (Continued)

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Hawkins & Armstrong 1954

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FIGURE 2.1.2.4.10.1 Logarithm of vapor pressure versus reciprocal temperature for β-pinene.
### TABLE 2.2.1
Summary of physical properties of aliphatic and cyclic hydrocarbons

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<th>b.p.°C</th>
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* Assuming $\Delta S_{\text{ fus }} = 56 \text{ J/mol K.}$
### TABLE 2.2.2
Summary of selected physical-chemical properties of aliphatic and cyclic hydrocarbons at 25\(^{\circ}\)C

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<td>P(_L)/Pa</td>
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(Continued)
### TABLE 2.2.2 (Continued)

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* Vapor pressure exceeds atmospheric pressure, Henry’s law constant H/(Pa·m^3/mol) = 101325 Pa/C S mol/m^3.
### Table 2.2.3
Suggested half-life classes of hydrocarbons in various environmental compartments at 25°C

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where,

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**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.


Aliphatic and Cyclic Hydrocarbons


Parks, G.S., Huffman, H.M. (1931) Some fusion and transition data for hydrocarbons.


3.1 List of Chemicals and Data Compilations

3.1.1 Mononuclear aromatic hydrocarbons

- Benzene ......................................................... 407
- Toluene .......................................................... 425
- Ethylbenzene ...................................................... 439
- o-Xylene .......................................................... 450
- m-Xylene .......................................................... 459
- p-Xylene .......................................................... 467
- 1,2,3-Trimethylbenzene ......................................... 476
- 1,2,4-Trimethylbenzene .......................................... 481
- 1,3,5-Trimethylbenzene .......................................... 486
- n-Propylbenzene .................................................. 493
- Isopropylbenzene .................................................. 500
- 1-Ethyl-2-methylbenzene (o-Ethyltoluene) .................. 505
- 1-Ethyl-3-methylbenzene (m-Ethyltoluene) .................. 508
- 1-Ethyl-4-methylbenzene (p-Ethyltoluene) .................. 512
- 1-Isopropyl-4-methylbenzene (p-Cymene) ................... 516
- n-Butylbenzene .................................................... 520
- Isobutylbenzene .................................................... 525
- sec-Butylbenzene ................................................... 528
- tert-Butylbenzene .................................................. 532
- 1,2,3,4-Tetramethylbenzene ..................................... 536
- 1,2,3,5-Tetramethylbenzene ..................................... 539
- 1,2,4,5-Tetramethylbenzene ..................................... 542
- Pentamethylbenzene .............................................. 545
- Pentybenzene ....................................................... 547
- Hexamethylbenzene ............................................... 550
- n-Hexylbenzene ..................................................... 553
- Heptylbenzene ...................................................... 557
- n-Octylbenzene ...................................................... 559
- Nonylbenzene ....................................................... 562
- Decylbenzene ....................................................... 564
- Undecylbenzene ...................................................... 567
- Dodecylbenzene ..................................................... 569
- Tridecylbenzene ..................................................... 572
- Tetradecylbenzene .................................................. 574
- Styrene ............................................................. 576
- α-Methylstyrene ..................................................... 582
- β-Methylstyrene ...................................................... 584
- o-Methylstyrene ..................................................... 586
- m-Methylstyrene ..................................................... 588

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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: C₆H₆
Molecular Weight: 78.112
Melting Point (°C):
5.49 (Lide 2003)
Boiling Point (°C):
80.09 (Lide 2003)
Density (g/cm³ at 20°C):
0.8765 (Weast 1982–1983)
Molar Volume (cm³/mol):
89.1 (20°C, calculated from density)
96.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
33.843, 30.726 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion ∆Hfus (kJ/mol):
9.916 (Tsonopoulos & Prausnitz 1971)
9.866 (Riddick et al. 1986)
9.87 (exptl., Chickos et al. 1999)
Entropy of Fusion ∆Sfus (J/mol K):
35.564 (Tsonopoulos & Prausnitz 1971)
35.4, 44.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F:
1.0
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1850 (30°C, 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°C, Arnold et al. 1958)
S/(wt.%) = 0.1806 – 0.001095·(t/°C) + 3.170 × 10⁻³·(t/°C)²; temp range 5–45°C (shake flask-UV, Arnold et al. 1958); or
S/(wt.%) = 0.1784 – 0.0007436·(t/°C) + 1.1906 × 10⁻⁵·(t/°C)² + 1.217 × 10⁻⁷·(t/°C)³; temp range 5–45°C (shake flask-UV, Arnold et al. 1958)
1800* (24°C, shake flask-UV, measured range 0.8–64.5°C, Alexander 1959)
1890 (35°C, shake flask-UV spectrophotometry, Hine et al. 1962)
1742* (shake flask-UV, measured range 17–63°C, Franks et al. 1963)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

12654  (Hg manometer, Hovorka & Dreisbach 1934)
9960*  (20°C, manometer, measured range 0–50°C, Stuckey & Saylor 1940)

log (P/mmHg) = 7.12491 – 1323.06/(T/K) + 0.6838 (T/K) \times 10^3; temp range 0.2–25.8°C (generator column-HPLC/UV, May et al. 1978, 1980)

S/(μg/kg) = [1833 + 0.3166·(t/°C)^2 – 0.6838·(t/°C)^3] \times 10^3; temp range 0–55°C (Ueda et al. 1978)

\log x = 424.544/(T/K)^2 – 2955.82/(T/K) + 1.6606; temp range 0–55°C (Ueda et al. 1978)

ln (1/x) = –6.191 + 14.03·[(T/K)/562.2]–1 – 3.511·[(T/K)/562.2]–2; temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994a)

ln x = –15.54467 – 1442.4276/(T/K) – 3.283 \times 10^{-5}·(T/K)^2; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

ln x = –180.368 + 7524.83/(T/K) + 25.8585·ln (T/K); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)
11700* (23.7°C, ebulliometry-manometer, measured range 14.5–80.9°C, Willingham et al. 1945)

log (P/mmHg) = 6.89324 – 1203.835/(219.924 + t/°C); temp range 14.5–80.9°C (ebulliometry-manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

1332* (26.1°C, summary of literature data, Stull 1947)

11720* (23.2°C, ebulliometry, measured range 10.9–80.9°C, Forziati et al. 1949)

log (P/mmHg) = 6.91210 – 1214.645/(221.205 + t/°C); temp range 10.9–80.9°C (ebulliometry-manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

12690 (interpolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.90565 – 1211.033/(220.79 + t/°C); temp range 0–160°C (Antoine eq. for liquid state, Dreisbach 1955)


545800* (146.85°C, ebulliometry, measured range 146.85–286.85°C, Ambrose et al. 1967)

32045* (46.85°C, summary of literature data, temp range 46.85–286.85°C, Ambrose et al. 1970)

12700* (extrapolated-Antoine eq., Zwolinski & Wilhoit, 1971)

log (P/mmHg) = 6.90565 – 1211.033/(220.790 + t/°C); temp range –11.6 to 103.92°C (Antoine eq., Zwolinski & Wilhoit 1971)

12680 (extrapolated, Antoine eq., Boublik et al. 1973; 1984)

log (P/mmHg) = [–0.2185 × 10254.2/(T/K)] + 9.5560; temp range –58 to –30°C (Antoine eq., Weast 1972–73)

12640* (average, ebulliometry-bubble cap boilers, measured range 290–378 K, Ambrose 1981)

12100 (gas saturation-GC, Politzki et al. 1982)

log (P/atm) = (1 – 353.214/T) × 10^(0.832632 – 6.72598 × 10^4·T + 6.38324 × 10^7·T^2); T in K, temp range 280.0–562.6 K (Cox vapor pressure eq., Chao et al. 1983)

12690, 12680 (interpolated-Antoine equations, Boublik et al. 1984)

log (P/mmHg) = 6.01905 – 1204.637/(220.069 + t/°C); temp range 21.2–105°C (Antoine eq. from reported exptl. data of Ambrose 1981, Boublik et al. 1984)

log (P/kPa) = 6.01788 – 1203.677/(219.904 + t/°C); temp range 14.5–80.9°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

12690 (extrapolated, Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 9.1097 – 1885.9/(244.2 + t/°C); temp range –12 to 3°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.90565 – 1211.033/(220.79 + t/°C); temp range 8–103°C (Antoine eq., Dean 1985, 1992)

12716 (headspace-GC, Hussam & Carr 1985)

log (P/kPa) = 6.02232 – 1206.33/(219.9 + t/°C); temp range not specified (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 10.0091 – 2836/(25.31 + T/K); temp range 223–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 8.45261 – 1986.69/(−23.089C + T/K); temp range 218–279 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.01907 – 1204.682/(−53.072 + T/K); temp range 279–377 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 6.06832 – 1236.034/(−48.99 + T/K); temp range 353–422 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/kPa) = 6.3607 – 1466.083/(−15.44 + T/K); temp range 420–502 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P/kPa) = 7.51922 – 2809.514/(171.489 + T/K); temp range 501–562 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

13100* (gas saturation, measured range –15.4 to 40°C, Liu & Dickhut 1994)

log (P/mmHg) = 31.7718 – 2.7254 × 10^4/(T/K) – 8.4442·log (T/K) – 5.3534 × 10^-5·(T/K) + 2.7187 × 10^-6·(T/K)^2; temp range 279–562 K (vapor pressure eq., Yaws 1994)

log (P/kPa) = 6.02994 – 1211.033/(T/K) – 52.36; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional
data at other temperatures designated * are compiled at the end of this section):

- 653 (30°C, concn ratio-UV, Saylor et al. 1938)
- 576 (Taha et al. 1966)
- 442* (20.06°C, headspace-GC, Brown & Wasik 1974)

\[
\ln [H/(Pa m^3/mol)] = 21.26071 - 4445.58/(T/K); \text{ temp range } 4.5-20°C \quad \text{(regression eq. of exptl. data of Brown and Wasik 1974, Shi & Ma 2000)}
\]

- 555, 530 (calculated as 1/K_{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-conc. ratio-UV, measured range 10–30°C, Green & Frank 1979)

\[
\ln (H/\text{atm}) = 8.58 - 1852.308/(T/K); \text{ temp range } 10-30°C \quad \text{(shake flask-concn-UV, Green & Frank 1979)}
\]

- 544 (20°C, EPICS-GC, calculated-P/C, Yurteri et al. 1987)
- 535; 588; 554; 555 (EPICS-GC/FID; batch air stripping-GC; calculated P/C; direct concentration ratio; calculated-UNIFAC, Ashworth et al. 1988)
- 535* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
- 558* (infinite activity coeff. $\gamma_\infty$ from solubility measurement, Abraham et al. 1990)
- 564* (extrapolated from equilibrium headspace-GC data, measured range 40–80°C, Ettre et al. 1993)

\[
\ln (1/K_{AW}) = -2.1678537 + 836.2228/(T/K); \text{ temp range: } 45–80°C \quad \text{(equilibrium headspace-GC measurements, Ettre et al. 1993)}
\]

- 569 (infinite activity coeff. $\gamma_\infty$ in water determined by inert gas stripping-GC, Li et al. 1993)
- 504 (concentration ratio, Keeley et al. 1993)
- 544 (headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)
- 488 (23°C, gas stripping-IR, Nielsen et al. 1994)
- 481* (EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)

\[
\ln K_{AW} = -3640/(T/K) + 0.00786\cdot Z + 10.577; \text{ with } Z \text{ salinity } 0–35.5‰, \text{ temp range: } 2–35°C \quad \text{(EPICS-GC/FID, Dewulf et al. 1995)}
\]

- 538* (headspace equilibrium-GC, Peng & Wan 1997)
- 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 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
log $K_{AW} = 5.053 - 1693/(T/K)$ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

538* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)

$\ln K_{AW} = 8.1648 - 2889.4/(T/K)$; temp range 15–40°C (SPME-GC, Bierwagen & Keller 2001)

573.4* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)

$\ln K_{AW} = 10.01 - 3430.4/(T/K)$; temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)

514–606 (27°C, headspace equilibrium-GC, at different solute concn: 0.48–19.1 mg/L, measured temp range 300–315 K, Cheng et al. 2003)


$\ln (1/K_{AW}) = 11.663 - 3920/(T/K)$; temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyński 2003)

Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°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, 2.03, 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-k’ 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’ correlation, Rapaport & Eisenreich 1984)

2.13 (generator column-GC/ECID, 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* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.90* (20.29°C, from GC-determined $\gamma^\infty$ in octanol, measured range 20.290–50.28°C, Gruber et al. 1997)

2.80 (head-space GC-FID both phases, Abraham et al. 2001)

Bioconcentration Factor, log 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 (algae, fish, Freitag et al. 1984)

1.48 (algae, Geyer et al. 1984)

0.63 (gold fish, Ogata et al. 1984)

Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°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)

1.06, 1.65 (shake flask-UV, calculated-M.O. indices, Rogers & Cammarata 1969)

2.13 (calculated-fragment const., Rekker 1977)

2.13, 1.56, 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-k’ 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’ correlation, Rapaport & Eisenreich 1984)

2.13 (generator column-GC/ECID, 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* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)
Sorption Partition Coefficient, \( \log K_{OC} \) at 25°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; 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 B 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 horizon OC 3.25%; Oshtemo soil B horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
1.89 (aquifer material with \( f_{OC} \) of 0.006 and measured partition coeff. \( K_p = 0.47 \text{mL/g.} \), 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-\( K' \) 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 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon \( f_{OC} = 4.12\% \), 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 mmol/kg at pH 7, batch equilibrium-sorption isotherm, Li et al. 2000)
1.64, 1.58, 1.78 (soils: organic carbon OC \( \geq 0.1\% \), OC \( \geq 0.5\% \), 0.1 \( \leq \) OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, \( \log K_{OM} \):

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 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 horizon OM 4.38%; Oshtemo soil B 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 isotherm-GC, Rutherford & Chiou 1992)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization: \( t_{1/2} = 4.81 \text{ h from water depth of 1 m} \) (calculated, Mackay & Leinonen 1975; Haque et al. 1980); \( k = 0.03 \text{ d}^{-1} \) with \( t_{1/2} = 23 \text{ d} \) in spring at 8–16°C, \( k = 0.22 \text{ d}^{-1} \) with \( t_{1/2} = 31 \text{ d} \) in summer at 20–22°C, \( k = 0.054 \text{ d}^{-1} \) with \( t_{1/2} = 13 \text{ d} \) in winter at 3–7°C during the periods when volatilization appears to dominate, and \( k = 0.101 \text{ d}^{-1} \) with \( t_{1/2} = 6.9 \text{ d} \) with \( \text{HgCl}_2 \) in September 9–15, 1980 in marine mesocosm experiments (Wakeham et al. 1983);
\( t_{1/2} \sim 27 \text{ h from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s is 2.7 h at 20°C} \) (Lyman et al. 1982).
Mononuclear Aromatic Hydrocarbons

Photolysis: atmospheric photolysis $t_{1/2} = 2808–16152$ h, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991); aqueous photolysis $t_{1/2} = 2808–16152$ h, based on measured photolysis half-lives in deionized water (Hustert et al. 1981; Howard et al. 1991); reaction rate constants, $k = 8.64 \times 10^{-4}$ h$^{-1}$ in air, and $k = 1.8 \times 10^{-4}$ h$^{-1}$ in water (Mackay et al. 1985).

Oxidation: rate constant $k$; and gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

$k_{OH} = 1.24 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH(3P)} = 0.24 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction of O($^3$P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} \leq 2.3 \times 10^9$ L mol$^{-1}$ s$^{-1}$ with $t_{1/2} \geq 5.1$ h; $k_{OH(3P)} = (0.144 \pm 0.2) \times 10^9$ L mol$^{-1}$ s$^{-1}$ with O($^3$P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (1.20 \pm 0.15) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OI} = 0.85 \times 10^9$ L mol$^{-1}$ s$^{-1}$ with t$_{1/2}$ = 2.4–24 h (Darnall et al. 1976)

$k_{OH} = 0.85 \times 10^9$ L mol$^{-1}$ s$^{-1}$ at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = 1.26 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 23.8°C, with an atmospheric lifetime of 9.1 d (Edney et al. 1986)

$k_{OH} = 1.14 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 239–354 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{OH} = 2.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{OH} = 1.19 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{OH} = 1.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{OH} = 1.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{OH(calc)} = 1.90 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C, with an atmospheric lifetime of 9.1 d (Edney et al. 1986)

$k_{OH(obs.)} = 1.90 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH(calc)} = 2.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{OH} = 1.26 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 23.8°C, with an atmospheric lifetime of 9.1 d (Edney et al. 1986)

$k_{OH} = 1.14 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp., measured range 239–354 K (flash photolysis-resonance fluorescence, Witte et al. 1986)

$k_{OH(calc)} = 2.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH(calc)} = 1.28 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = (1.29 \pm 1.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K, measured range 234–438 K (flash photolysis-resonance fluorescence, Wallington et al. 1987)

$k_{OH} < 0.01 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH} = 1.28 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{NO3} < 3.2 \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson & Aschmann 1988)

$k_{OH} = 1.40 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 1.23 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1990)

$k_{OH(calc)} = 1.51 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

$t_{1/2} = 6$ d in estuarine water (estimated, Lee & Ryan 1976)

$t_{1/2}(aq.\, aerobio) = 120–384$ h, based on seawater dieaway test data (Van der Linden 1978) and river dieaway data (Vaishnav & Babeu, 1987; Howard et al. 1991)

$k = 4.58 \times 10^{-3}$ h$^{-1}$ in water (Lee & Ryan 1979; Mackay et al. 1985)

$k = 0.2$ yr$^{-1}$ with $t_{1/2} = 110$ d (Zoeteman et al 1981; Olsen & Davis 1990)

$k = 0.5$ d$^{-1}$ significant degradation in favourable aerobic environment (Tabak et al. 1981; Mills et al. 1982)

$t_{1/2}(aq.\, anaerobio) = 2688–17280$ h, based on unacclimated aqueous anaerobic biodegradation screening test data (Horowitz et al. 1982; Howard et al. 1991)

$k = 0.12$ d$^{-1}$ in river water (estimated, Bartholomew & Pfaender 1983; quoted, Battersby 1990)

$t_{1/2} = 8.6$ d in activated sludge (estimated, Freitag et al. 1985, quoted, Anderson et al. 1991)

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k = 0.025 d^{-1} with t_{1/2} = 28 d in groundwater, k = 0.044 d^{-1} with t_{1/2} = 16 d in Lester River with nutrient and microbial addition, and k = 0.082 d^{-1} with t_{1/2} = 8 d in Superior harbor waters (Vaishnav & Babeu 1987)
t_{1/2}(aerobic) = 5 d, t_{1/2}(anaerobic) = 110 d in natural waters (Capel & Larson 1995)
k = 0.58 d^{-1} associated with microbial population growth initially followed by a slower second phase with k = 0.12 d^{-1} degradation by \textit{P. aeruginosa} is a two-stage process (Kim et al. 2003).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Constants or Half-Lives:
t_{1/2} = 0.5 d for elimination from eels, 0.5 d (Ogata & Miyake 1978).

Half-Lives in the Environment:

**Air:** t_{1/2} \geq 5.1 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);
t_{1/2} = 2.4–24 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);
t_{1/2} = 50.1–501 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 d, > 4 yr and > 4.5 yr for reactions with OH radical, NO_3 radical and O_3, respectively (Atkinson 2000).

**Surface Water:**
t_{1/2} = 4.81 h, based on evaporation loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975)
biodegradation t_{1/2} \sim 6 d in estuarine water (Lee & Ryan 1976)
t_{1/2} = 120–384 h, based on unacclimated aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991);
t_{1/2} = 23 d at 8–16°C in the spring, t_{1/2} = 3.1 d at 20–22°C in the summer and t_{1/2} = 13 d at 3–7°C in the winter,
and t_{1/2} = 6.9 d with HgCl_2 in September 9–15 from mesocosm experiments (Wakeham et al. 1983).

**Ground water:** t_{1/2} \sim 1 yr from persistence observed in the groundwater of Netherlands (Zoeteman et al. 1981),
t_{1/2} = 240–17280 h, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991).

**Soil:** t_{1/2} = 120–384 h, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Vaishnav & Babeu 1987; Howard et al. 1991);
t_{1/2} < 10 d (Ryan et al. 1988);
t_{1/2} = 365 d, assumed first-order biological/chemical degradation in the soil (Jury et al. 1990);
disappearance t_{1/2} < 2 d for test soils (Anderson et al. 1991).

**Biota:**
TABLE 3.1.1.1
Reported aqueous solubilities of benzene at various temperatures and reported temperature dependence equations

\[ R \ln x = -\left[\Delta H_{\text{ fus}}/(T/K)\right] + (0.000408)(T/K) - 291.15 + b(T/K) \]  
\[ 'S/(\mu g/kg) = a + b t^3 + c t^2 + d \]  
\[ \ln x = A - B/T(K) \]  
\[ \ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_o, T_o = 298.15 \text{ K} \]

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\( \Delta H_{\text{ fus}}/(kJ \text{ mol}^{-1}) = 27.3 \)

\( \Delta H_{\text{ fus}}/(kJ \text{ mol}^{-1}) = 2.27 \) at 25°C

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### TABLE 3.1.1.1 (Continued)

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- Temp dependence eq. 2  
- Given in May et al. 1978b and May 1980

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   [vapor saturation-UV]  

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- ∆Hsol/(kJ mol⁻¹) = 3.69
- at 25°C

Sanemasa et al. 1982  
   [vapor saturation-UV]  

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- ∆Hsol/(kJ mol⁻¹) = 2.07
- at 25°C

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FIGURE 3.1.1.1 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

- $\log P = A - B/(T/K)$
- $\log P = A - B/(C + t/°C)$
- $\log P = A - B/(C + T/K)$
- $\log P = A - B/(T/K) - C\cdot\log (T/K)$
- $\log P = A - B/(T/K) - C\cdot\log (T/K) + D\cdot P/(T/K)^2$

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TABLE 3.1.1.2 (Continued)

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**FIGURE 3.1.1.2** Logarithm of vapor pressure versus reciprocal temperature for benzene.

- experimental data
- Stull 1947
- Zwolinski and Wilhoit 1971

Benzene: vapor pressure vs. 1/T

- b.p. = 80.09 °C
- m.p. = 5.49 °C
TABLE 3.1.1.3
Reported Henry's law constants of benzene at various temperatures and reported temperature dependence equations

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \\
\ln (1/K_{AW}) &= A - B/(T/K) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \\
\ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) \\
K_{AW} &= A - B \cdot (T/K) + C \cdot (T/K)^2
\end{align*}
\]

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**enthalpy of volatilization:**

$$\Delta H_{vol}/(kJ\cdot mol^{-1}) = 32.2$$

at 20°C

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FIGURE 3.1.1.1.3 Logarithm of Henry’s law constant versus reciprocal temperature for benzene.

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change in enthalpy:  
\( \Delta H_{\text{OW}}/(\text{kJ mol}^{-1}) = 1.7 \)  
\((-8.3\text{ to } 11.8)\)  
entalphy of transfer  
\( \Delta H_{\text{OA}}/(\text{kJ mol}^{-1}) = 8.1 \)  
\((-1.9\text{ to } 18.2)\)
FIGURE 3.1.1.4 Logarithm of $K_{OW}$ and $K_{OA}$ 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: C₇H₈, C₆H₅CH₃
Molecular Weight: 92.139
Melting Point (°C):
  −94.95  (Lide 2003)
Boiling Point (°C):
  110.63  (Lide 2003)
Density (g/cm³ at 20°C):
  0.8669  (Weast 1982–83)
Molar Volume (cm³/mol):
  106.3  (20°C, calculated from density)
  118.2  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
Enthalpy of Fusion \( \Delta H_{ fus } \) (kJ/mol):
  6.636  (Riddick et al. 1986)
  6.62  (exptl., Chickos et al. 1999)
Entropy of Fusion \( \Delta S_{ fus } \) (J/mol K):
  37.15, 45.0  (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C or indicated. Additional data at other temperatures designated * are compiled at the end of this section):
  470  (16°C, shake flask, Fühner, 1924)
  570  (30°C, 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°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  (21°C, shake flask-GC, Chey & Calder 1972)
  530*  (shake flask-GC, measured range 5–45°C, Pierotti & Liabastre 1972)
  573*  (shake flask-GC, Polak & Lu 1973)
  517  (shake flask-GC, Mackay & Wolkoff 1973)
  488; 563  (shake flask-titration, shake flask-cloud point, Sada et al. 1975)
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<tr>
<td>558*</td>
<td>(shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)</td>
</tr>
<tr>
<td>(\ln x = -221.739 + 9274.79/(T/K) + 31.8721 \cdot \ln (T/K)); temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)</td>
<td></td>
</tr>
</tbody>
</table>

**Vapor Pressure (Pa at 25°C and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section):**

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>920*</td>
<td>(0°C, mercury manometer, measured range –9.70 to 0°C, Linder 1931)</td>
</tr>
<tr>
<td>3786*</td>
<td>(Hg manometer measurements, Pitzer &amp; Scott 1943)</td>
</tr>
<tr>
<td>(\log (P/mmHg) = -2866.53/(T/K) - 6.7 \log (T/K) + 27.6470); temp range: 0–50°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer &amp; Scott 1943)</td>
<td></td>
</tr>
<tr>
<td>6357*</td>
<td>(35.366°C, ebulliometry, measured range 35.366–111.509°C, Willingham et al. 1945)</td>
</tr>
<tr>
<td>(\log (P/mmHg) = 6.95337 - 1343.943/(219.377 + t/°C)); temp range 35.4–111.5°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)</td>
<td></td>
</tr>
<tr>
<td>2666*</td>
<td>(18.4°C, summary of literature data, temp range –16.7 to 110.6°C, Stull 1947)</td>
</tr>
<tr>
<td>6886*</td>
<td>(35.504°C, ebulliometry, measured range 35.504–111.545°C, Forziati et al. 1949)</td>
</tr>
<tr>
<td>(\log (P/mmHg) = 6.95508 - 1345.087/(219.516 + t/°C)); temp range 35.5–111.5°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)</td>
<td></td>
</tr>
<tr>
<td>3792</td>
<td>(calculated from det. data, Dreisbach 1955)</td>
</tr>
<tr>
<td>(\log (P/mmHg) = 6.95334 - 1343.943/(219.377 + t/°C)); temp range 20–200°C (Antoine eq. for liquid state, Dreisbach 1955)</td>
<td></td>
</tr>
<tr>
<td>256200*</td>
<td>(146.85°C, ebulliometry, measured range 146.85–306.85°C, Ambrose et al. 1967)</td>
</tr>
<tr>
<td>48898*</td>
<td>(86.85°C, compiled data, temp range 86.85–306.85°C, Ambrose et al. 1970)</td>
</tr>
<tr>
<td>3792*</td>
<td>(interpolated, Antoine eq., Zwolinski &amp; Wilhoit 1971)</td>
</tr>
</tbody>
</table>
\[ \log (P/\text{mmHg}) = 6.95464 - 1344.80/(219.482 + t/\degree C); \text{ temp range; 6.36–136.42}\degree C (\text{Antoine eq., Zwolinski \\& Wilhoit 1971}) \]

\[ \log (P/\text{mmHg}) = [-0.2185 \times 9368.5/(T/K)] + 8.3300; \text{ temp range –92 to –15}\degree C (\text{Antoine eq., Weast 1972–73}) \]

\[ \log (P/\text{mmHg}) = [-0.2185 \times 8586.5/(T/K)] + 8.719392; \text{ temp range –26.7 to 319}\degree C (\text{Antoine eq., Weast 1972–73}) \]

\[ 2904^* (19.99\degree C, \text{differential capacitance gauge, measured range 0–49.26}\degree C, \text{Munday et al. 1980}) \]

\[ \log (P/\text{atm}) = (1 – 383.737/T) \times 10^{0.837122 – 6.48791 \times 10^4 \cdot T + 5.91293 \times 10^7 \cdot T^2}; T \text{ in K, temp range 245.0–590.0 K (Cox vapor pressure eq., Chao et al. 1983}) \]

\[ \log (P/\text{atm}) = 6.08436 – 1347.62/(219.976 + t/\degree C); \text{ temp range 35.37–111.5}\degree C (\text{Antoine eq., Riddick et al. 1986}) \]

\[ \log (P/\text{atm}) = 6.1258 – 1376.61/(–51.1 + T/K); \text{ temp range 210–219 K (liquid, Antoine eq.-II, Stephenson \\& Malanowski 1987}) \]

\[ \log (P/\text{atm}) = 6.40815 – 1615.834/(–15.897 + T/K); \text{ temp range 440–531 K (liquid, Antoine eq.-IV, Stephenson \\& Malanowski 1987}) \]

\[ \log (P/\text{atm}) = 7.65383 – 3153.235/(188.566 + T/K); \text{ temp range 383–445 K (liquid, Antoine eq.-III, Stephenson \\& Malanowski 1987}) \]

\[ \log (P/\text{atm}) = 6.1273 – 1391.005/(–49.747 + T/K); \text{ temp range 273–295 K (liquid, Antoine eq.-VI, Stephenson \\& Malanowski 1987, selected, Shi & Ma 2000}) \]

\[ \log (P/\text{atm}) = 5.133 – 3024/(T/K); \text{ temp range 10–30\degree C (EPICS measurements, Ashworth et al. 1988}) \]

\[ \log (P/\text{atm}) = 6.03 + 2198/(T/K); \text{ temp range 40–80\degree C, Kolb et al. 1992}) \]

Henry’s Law Constant (Pa m^3/mol at 25\degree C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

474* (headspace-GC, Brown & Wasik 1974)

527 (headspace-GC, Vitenberg et al. 1975)

673 (batch air stripping-GC, Mackay et al. 1979)

625* (23.0\degree C, equilibrium cell-concn ratio-GC/FID, Leighton & Calo 1981)

\[ \ln (k_H/\text{atm}) = 18.46 – 3751/(T/K); \text{ temp range:1.0–23.0}\degree C (\text{equilibrium cell-concn ratio}, Leighton & Calo 1981) \]

628* (vapor-liquid equilibrium-GC., Sanemasa et al. 1981)

664* (vapor-liquid equilibrium, Sanemasa et al. 1982)

647 (EPICS-GC, Garbarnini & Lion 1985)

634* (20\degree C, headspace-GC, measured range 20–46\degree C, Schoene & Steinhanses 1985)

601 (gas stripping-GC, Warner et al. 1987)

594 (20\degree C, EPICS, Yurteri et al. 1987)

651* (EPICS-GC, Ashworth et al. 1988)

\[ \ln [H/(\text{atm m^3/mol})] = 5.133 – 3024/(T/K); \text{ temp range 10–30\degree C (EPICS measurements, Ashworth et al. 1988}) \]

652 (infinite activity coeff. \( \gamma \) from solubility measurement, Abraham et al. 1990)

644 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

933* (40\degree C, static headspace-GC, measured range 40–80\degree C, Kolb et al. 1992)

\[ \ln (1/K_{AW}) = –6.03 + 2198/(T/K); \text{ temp range 40–80\degree C (equilibrium headspace-GC measurements, Kolb et al. 1992}) \]

1116* (45\degree C, headspace-GC, measured range 45–80\degree C, Ettre et al. 1993)

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\[ \log \left( \frac{1}{K_{\text{AW}}} \right) = -2.5323790 + \frac{928.3536}{(T/\text{K})}; \text{ temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)} \]

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 (23°C, 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)

\[ \ln K_{\text{AW}} = \frac{-4064}{(T/\text{K})} + 0.00834 \cdot Z + 12.150; \text{ with } Z \text{ salinity 0–35.5‰, temp range 2–35°C, (EPICS-GC/FID, Dewulf et al. 1995)} \]

541 (20°C, 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)

\[ \ln K_{\text{AW}} = 7.94 - 1621/(T/\text{K}); \text{ temp range 15–45°C (headspace equilibrium-GC, Peng & Wan 1997)} \]

478 (headspace-GC, Peng & Wan 1998)

\[ \ln K_{\text{AW}} = 7.89 - 1565/(T/\text{K}); \text{ temp range 0–45°C (seawater with salinity of 36‰, headspace-GC, Peng & Wan 1998)} \]

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 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log \( K_{\text{AW}} = 5.271 - 1745/(T/\text{K}) \) (van't Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

647.5* (EPICS-SPME, measured range 2–60°C, Görgényi et al. 2002)

\[ \ln K_{\text{AW}} = 11.25 - 3770.4/(T/\text{K}); \text{ temp range 2–60°C (EPICS-SPME method, Görgényi et al. 2002)} \]

556–574 (27°C, solid-phase microextraction-GC, solute concn 0.47–19.21 mg/L, measured range 15–40°C, Cheng et al. 2003)


\[ \ln (1/K_{\text{AW}}) = 11.926 - 3977/(T/\text{K}); \text{ temp range 10–25°C, headspace-GC, Bakierowska & Trzeszczyński 2003} \]

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \) at 25°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 (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-k’ correlation, Hafkanscheid & Tomlinson 1983b)

2.11–2.80, 2.65 (range, mean; shake flask method, Eadsforth & Moser 1983)

2.51–3.06, 2.88 (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)
Mononuclear Aromatic Hydrocarbons

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 ± 0.05, 2.786 ± 0.005 (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 ± 0.02 (HPLC-k' correlation, Poulson et al. 1997)
2.32* (24.8°C, EPICS-GC, measured range 2.2–24.8°C, Dewulf et al. 1999)

Octanol/Air Partition Coefficient, log KoA at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:
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 (activated sludge, algae, fish, Freitag et al. 1985)
1.99 (S. capricornutum, Herman et al. 1991)

Sorption Partition Coefficient, log KOC at 25°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 Al2O3, 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 (Sapsucker Woods humic acid, Sapsucker Woods fulvic acid, tannic acid, lignin, zein, cellulose, Aldrich humic acid, headspace equilibrium, Garbarnini & Lion 1986)
1.91, 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 (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 B 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 B horizon, OC 0.44%, batch equilibrium, Lee et al. 1989)
3.03, 2.90 (organic cations HDTMA treated soils: St. Clair soil B horizon OC 3.25%; Oshtemo soil B horizon OC 0.83%, batch equilibrium-adsorption isotherm, Lee et al. 1989)
2.01 (aquifer material with fOC = 0.006 and measured partition coeff. Kp = 0.61 mL/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-k' 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, 2.40, 2.31, 2.34 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon fOC = 4.12%, EPICS-GC/FID, Dewulf et al. 1999)
1.89, 2.00, 1.79 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
Sorption Partition Coefficient, log $K_{OM}$:

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 B 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 horizon, OM 0.88%, batch equilibrium, Lee et al. 1989)

2.89; 2.74 (organic cations HDTMA treated soils: St. Clair soil B horizon OM 4.38%; Oshtemo soil B horizon OM 1.12%, batch equilibrium-adsorption isotherm, Lee et al. 1989)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 5.18$ h from water depth of 1-m (Mackay & Leinonen 1975; Haque et al. 1980);

$k = 0.043 \text{ d}^{-1}$ with $t_{1/2} = 16$ d in spring at 8–16°C, $k = 0.0463 \text{ d}^{-1}$ with $t_{1/2} = 1.5$ d in summer at 20–22°C, $k = 0.053 \text{ d}^{-1}$ with $t_{1/2} = 13$ d in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.088 \text{ d}^{-1}$ with $t_{1/2} = 7.6$ d with HgCl$_2$, in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

evaporation $t_{1/2} \sim 2.9$ d from a river of 1-m depth with wind speed of 3 m/s and water current of 1 m/s at 20°C (Lyman et al. 1982);

estimated $t_{1/2} = 1$ and 4 d for evaporation from a river and lake, respectively (Howard 1990).

Photolysis: not environmentally significant or relevant (Mabey et al. 1982);

$k \approx 3.39 \times 10^{-3} \text{ h}^{-1}$ with H$_2$O$_2$ under photolysis at 25°C in F-113 solution and with HO$_2$ in the gas (Dilling et al. 1988); $t_{1/2} < 0.25$ 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, $k_{OH}$ for reaction with OH radical, $k_{O_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

$k_{OH} = (2.5 \pm 0.9) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 4.6$ h; $k_{O_3}$ was $(0.450 \pm 0.045) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ with O($^3$P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = 5.78 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{O_3} = 0.75 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction of O($^3$P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 3.6 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$, with $t_{1/2} = 2.4–24$ h at room temp. (Darnall et al. 1976)

$k_{OH}^* = (6.40 \pm 0.64) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = 6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{O_3} \leq 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K (Carter et al. 1981)

$k_{OH} = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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)

$k < 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 144 \text{ M}^{-1} \text{ h}^{-1}$ for RO$_2$ radical (Mabey et al. 1982)

$k_{O_3} = 160 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k_{OH} = 3.5 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 1.6$ d in the atmosphere (Mill 1982)

$k = (14 \pm 3) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.7 and 20–23°C (Hoigne & Bader 1983; Carter et al. 1981)

$k_{O_3} < 1.0 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.0006 \text{ d}^{-1}$; $k_{OH} = 6.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.6 d$^{-1}$ and $k_{O_3} = 3.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.0007 d$^{-1}$ at room temp. (review, Atkinson & Carter 1984)

$k_{O_3} = 1.8 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{OH}^* = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1985)

$k_{OH}(\text{calc}) = 5.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1985)

$k_{OH} = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 10–104$ h (Atkinson 1985; Howard 1991)

$k_{O_3} = 1.0 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $< 0.0006 \text{ d}^{-1}$; $k_{OH} = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.27 d$^{-1}$ and $k_{O_3} = 3.6 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.0007 d$^{-1}$ at room temp. (review, Atkinson 1985)

$k_{OH} = 6.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{OH} = 5.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 24.2°C, with a calculated atmospheric lifetime $\tau = 2.2$ d (Edney et al. 1986)
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\[ k_{\text{OH}}(\text{calc}) = 5.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]

\[ k_{\text{OH}}(\text{obs.}) = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \]

Atkinon (1987)

\[ k_{\text{NO}_3} = 6.46 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, \]

\[ k_{\text{OH}} = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K} \]

Atkinson et al. (1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

\[ k_{\text{O}_3} < 0.01 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]

\[ k_{\text{OH}} = 6.19 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \]

(relative rate method, Atkinson & Aschmann 1988)

\[ k_{\text{OH}}(\text{calc}) = 4.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]

(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°C with an initial concn of 2.22 \times 10^{-6} \text{ L/L} (Jamison et al. 1976)

\[ t_{\frac{1}{2}} = 90 \text{ d in uncontaminated estuarine water; and } t_{\frac{1}{2}} = 30 \text{ d in oil polluted water} \]

(Lee 1977)

k = 0.5 d^{-1}, significant degradation in aerobic environment (Tabak et al. 1981; Mills et al. 1982)

k = 0.07 yr^{-1} with \[ t_{\frac{1}{2}} = 39 \text{ d (Zoeteman et al. 1981; Olsen & Davis 1990)} \]

\[ t_{\frac{1}{2}}(\text{aq. aerobic}) = 1344–5040 \text{ h, based on anaerobic screening test data and anaerobic sediment grab sample data (Horowitz et al. 1982; Howard et al. 1991)} \]

\[ t_{\frac{1}{2}} = 9.5 \text{ d in activated sludge (estimated, Freitag et al. 1985; quoted, Anderson et al. 1991)} \]

\[ t_{\frac{1}{2}}(\text{aq. aerobic}) = 96–528 \text{ h, based on an acclimated seawater dieaway test (Howard et al. 1991)} \]

\[ t_{\frac{1}{2}}(\text{aerobic}) = 4 \text{ d, } t_{\frac{1}{2}}(\text{anaerobic}) = 56 \text{ d in natural waters (Capel & Larson 1995)} \]

\[ t_{\frac{1}{2}} = 31–220 \text{ h for toluene concn range from 0.5–200 \mu g/g in sandy loam soil and degradation rate } k = 1.76 \times 10^{-2} \text{ and 0.42 } \mu g g^{-1} h^{-1} \text{ for soil of 0.5 and 5.0 } \mu g/g \text{ respectively; } t_{\frac{1}{2}} = 172 \text{ and 165 h in sand and degradation rate } k = 1.05 \times 10^{-2} \text{ and 0.22 } \mu g g^{-1} h^{-1} \text{ of soil for toluene concn 0.5 and 5 } \mu g/g \text{ respectively in sand (Davis & Madsen 1996)} \]

Biotransformation: \[ 1.0 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1} \]

(Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

\[ t_{\frac{1}{2}} \sim 1.4 \text{ d elimination from eels in seawater (Ogata & Miyake 1978)} \]

Half-Lives in the Environment:

Air: \[ t_{\frac{1}{2}} = 4.6 \text{ h in ambient air based on reaction with OH radical at } \sim 300K (Doyle et al. 1975); \]

\[ t_{\frac{1}{2}} = 2.4–24 \text{ h based on rate of disappearance for the reaction with hydroxyl radicals (Darnall et al. 1976); } \]

photodecomposition \[ t_{\frac{1}{2}} = 6.8 \text{ h under simulated atmospheric conditions, with NO (Dilling et al. 1976); } \]

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)

\[ \tau = 2.2 \text{ d due to reaction with OH radical (Edney et al. 1986)} \]

summer daylight lifetime of 23 h due to reaction with OH radical (Altshuller 1991)

\[ t_{\frac{1}{2}} = 10–104 \text{ h, based on photooxidation in air (Howard et al. 1991); } \]

\[ \tau = 1.9 \text{ d, } \tau = 1.9 \text{ yr and } > 4.5 \text{ yr for reactions with OH radical, NO}_3 \text{ radical and O}_3 \text{ respectively (Atkinson 2000)} \]

Surface Water: \[ t_{\frac{1}{2}} = 5.55 \text{ h, based on evaporative loss at 25°C and 1-m depth of water (calculated, Mackay & Leinonen 1975; Haque et al. 1980); } \]

\[ \text{photooxidation } t_{\frac{1}{2}} = 321–1284 \text{ h in water, based on measured rate data for hydroxyl radical in aqueous solution (Dorfman & Adams 1973; Howard et al. 1991); } \]

\[ t_{\frac{1}{2}} = 16 \text{ d in spring at 6–16°C, } t_{\frac{1}{2}} = 1.5 \text{ d in summer at 20–22°C, } t_{\frac{1}{2}} = 13 \text{ d in winter at 3–7°C when volatilization dominates and } t_{\frac{1}{2}} = 7.9 \text{ d with HgCl}_2 \text{ in marine mesocosm experiments (Wakeham et al. 1983); } \]

\[ t_{\frac{1}{2}} = 96–528 \text{ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); } \]

Ground Water: \[ t_{\frac{1}{2}} = 0.3 \text{ yr from observed persistence in groundwater of Netherlands (Zoeteman et al. 1981); } \]

\[ t_{\frac{1}{2}} = 168–672 \text{ h, based on unacclimated grab sample data of aerobic soil from groundwater aquifers (Wilson et al. 1983; Swindoll et al. 1987; Howard et al. 1991); } \]

Soil: \[ t_{\frac{1}{2}} < 10 \text{ d (Ryan et al. 1988); } \]

\[ t_{\frac{1}{2}} = 5 \text{ d assumed first-order biological/chemical degradation in soil (Jury et al. 1990); } \]
reported lit. $t_{1/2} = 0.1 - 1.7$ d and 7 d in soil, measured disappearance $t_{1/2} < 2.0$ d from test soils (Anderson et al. 1991).

$t_{1/2}$ = 96–528 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

$t_{1/2}$ = 31, 57, 96 and 220 h with toluene concn range from 0.5, 5, 50 and 200 µg/g in sandy loam soil, $t_{1/2}$ = 172 and 165 h with toluene concn 0.5 and 5 µg/g, respectively, in sand (Davis & Madsen 1996).

Biot: $t_{1/2}$ = 10 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

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$\Delta_{\text{sol}} H/(\text{kJ mol}^{-1}) = 3.70$ at 25°C
### TABLE 3.1.1.2.1 (Continued)

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<td>Schwarz &amp; Miller 1980</td>
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<td>Sanemasa et al. 1981</td>
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\[ \Delta H_{sol}/(kJ \cdot mol^{-1}) = 1.70 \] at 25°C

3.

<table>
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\[ \Delta H_{sol}/(kJ \cdot mol^{-1}) = 0.37 \] at 25°C

\[ \Delta H_{sol}/(kJ \cdot mol^{-1}) = 3.0 \] at 25°C

### 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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \\
\ln P &= A - \frac{B}{T/K} \\
\log P &= A - \frac{B}{C + T/K} \\
\log P &= A - \frac{B}{C + T/K} - C \cdot \log (T/K) \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) + D \cdot \frac{P}{(T/K)^2} \\
\log P &= A - \frac{B}{T/K} - C \cdot (T/K) + D \cdot (T/K)^2
\end{align*}
\]

1. | Pitzer & Scott 1943 | Stull 1947 | Willingham et al. 1945 | Forziati et al. 1949 |
--- | --- | --- | --- |
| mercury manometer | summary of literature data | ebulliometry | ebulliometry |
| t/°C | P/Pa | t/°C | P/Pa | t/°C | P/Pa | t/°C | P/Pa |
| 0 | 900 | –16.7 | 133.3 | 35.366 | 6357 | 35.504 | 6386 |
| 12.5 | 1920 | –4.40 | 666.6 | 39.343 | 7654 | 39.437 | 7690 |
| 25 | 3786 | 6.40 | 1333 | 42.810 | 8962 | 45.997 | 10328 |
| 37.5 | 7026 | 18.4 | 2666 | 45.948 | 10303 | 48.894 | 11719 |
| 50 | 12266 | 31.8 | 5333 | 48.810 | 11700 | 52.848 | 13840 |
| eq. 4 | P/mmHg | 51.9 | 1337 | 57.293 | 16621 | 61.869 | 19942 |
| A | 27.6470 | 89.5 | 5329 | 66.079 | 23450 | 71.758 | 28976 |
| B | 2866.53 | 90.623 | 101325 | 71.738 | 28952 | 76.965 | 34924 |
| C | 6.70 | 110.6 | 101325 | 76.942 | 13818 | 83.230 | 43359 |
\[
\Delta H_v/(kJ \text{ mol}^{-1}) = 38.137 \quad \text{mp}^\circ/°C \quad –95
\]
\[
at 298 \text{ K}
\]

--- | --- | --- | --- |
| compiled data | compiled data | selected values | differential capacitance gauge |
| t/°C | P/Pa | t/°C | P/Pa | t/°C | P/Pa | t/°C | P/Pa |
| 6.375 | 1333 | 86.85 | 48898 | 6.36 | 1333 | 0.0 | 901.3 |
| 46.748 | 10666 | 106.85 | 90097 | 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 | 186.85 | 589400 | 40.308 | 7999 | 39.60 | 7743 |
|-------------------|---------------------|--------------------------|---------------------|
| compiled data     | compiled data       | selected values          | differential capacitance gauge |
| \( t/°C \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) |
| eq. 5 | \( P/mmHg \) | 206.85 | 845520 | 46.733 | 10666 | 49.26 | 11870 |
| A | 24.2765 | 226.85 | 1176900 | 51.940 | 13332 | 25.08 | 284.47 |
| B | 2.04294 | 286.85 | 2768000 | 75.644 | 33331 | 5541 | 623 |
| C | 306.85 | 3556300 | 80.863 | 39997 | 0.01055321 | 0 |
| D | 110.64 | 89.484 | 53329 | 96.512 | 66661 | 102.511 | 79993 |
| Ambrose et al. 1967 | ebulliometry | | | |
| \( t/°C \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) |
| 146.85 | 256200 | 110.64 | | | 199.22 | 1.051×10^{-3} |
| 166.85 | 396600 | 110.625 | 101325 | | 215.91 | 7.660×10^{-3} |
| 186.85 | 589400 | 25.0 | 3792 | | 234.88 | 5.001×10^{-2} |
| 206.85 | 845400 | | | | 254.64 | 0.252 |
| 226.85 | 1177100 | bp/°C | 110.625 | | 274.01 | 0.956 |
| 246.85 | 1597700 | eq. 2 | \( P/mmHg \) | | 278.99 | 1.305 |
| 266.85 | 2122200 | A | 6.95464 | | 284.17 | 1.764 |
| 286.85 | 2767600 | B | 1344.80 | | 294.13 | 3.090 |
| 306.85 | 3556800 | C | 219.482 | | 304.06 | 5.145 |
| | | | | | 314.03 | 8.257 |

\[ \Delta H_v/(kJ \text{ mol}^{-1}) = \]

\[ \log(P_{S}/Pa) \]

\[ \text{experimental data} \]

\[ \text{Stull 1947} \]

\[ \text{Zwolinski and Wilhoit 1971} \]

| eq. 5 | P/bar | at \( 25°C \) | 37.99 | 33.18 | 353.98 | 40.016 |
| A | 20.17980 | | 37.99 | 33.18 | 353.98 | 40.016 |
| B | 2640.04 | | | | | |
| C | 5.14885 | | | | | |
| D | 1434 | | | | | |

1 bar = 1 \times 10^5 Pa

**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

\[
\ln K_{AW} = A - \frac{B}{T/K} \quad (1) \quad \log K_{AW} = A - \frac{B}{T/K} \quad (1a)
\]

\[
\ln \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} \quad (2) \quad \log \left( \frac{1}{K_{AW}} \right) = A - \frac{B}{T/K} \quad (2a)
\]

\[
\ln [H/(\text{Pa m}^{3}/\text{mol})] = A - \frac{B}{T/K} \quad (3) \quad \ln [H/(\text{atm} \cdot \text{m}^{3}/\text{mol})] = A - \frac{B}{T/K} \quad (4a)
\]

\[
K_{AW} = A - B \cdot \left( \frac{T}{K} \right) + C \cdot \left( \frac{T}{K} \right)^2 \quad (5)
\]

1.  
**Brown & Wasik 1974**  
head space-GC  
Leighton & Calo 1981  
equilibrium cell-GC  
Sanemasa et al. 1981  
headspace-GC  
Koa & S. 1985  
vapor liquid-equilibrium  
eq. 1  

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\[ k_{\text{AW}} \text{ at atm} \]

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2.  
**Ashworth et al. 1988**  
Kolb et al. 1992  
Ettre et al. 1993  
Perllinger et al. 1993  

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\[ \text{eq. 4a} \]

<table>
<thead>
<tr>
<th>A</th>
<th>5.133</th>
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<tbody>
<tr>
<td>B</td>
<td>3024</td>
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3.  
**Robbins et al. 1993**  
Dewulf et al. 1995  
Turner et al. 1996  
Peng & Wan 1997  

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<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
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<th>H/(Pa m³/mol)</th>
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<td>25</td>
<td>652</td>
<td>2.0</td>
<td>175</td>
<td>11</td>
<td>376</td>
<td>15</td>
<td>391</td>
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<td>30</td>
<td>835</td>
<td>6.0</td>
<td>203</td>
<td>15</td>
<td>460</td>
<td>20</td>
<td>475</td>
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<td>40</td>
<td>1086</td>
<td>10</td>
<td>250</td>
<td>25</td>
<td>684</td>
<td>25</td>
<td>605</td>
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<td><strong>EPICS-GC</strong></td>
<td><strong>vapor phase-equilibrium</strong></td>
<td><strong>headspace-GC</strong></td>
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<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
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<td>(45)</td>
<td>1351</td>
<td>(18.2)</td>
<td>(424)</td>
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<td>(50)</td>
<td>1450</td>
<td>(25)</td>
<td>555</td>
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<tr>
<td>eq. 4a</td>
<td>(H/(\text{atm m}^3/\text{mol}))</td>
<td>eq 1</td>
<td>(K_{AW})</td>
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<td>B</td>
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<td>B</td>
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<th>Bakierowska &amp; T. 2003</th>
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<td><strong>EPICS-SPME method</strong></td>
<td><strong>headspace-GC</strong></td>
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<td>(t/°C)</td>
<td>(H/(\text{Pa m}^3/\text{mol}))</td>
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<td>2286</td>
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<td>(70)</td>
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**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

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OW}</th>
<th>log K_{OA}</th>
</tr>
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<tbody>
<tr>
<td>2.2</td>
<td>2.316</td>
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<td>6</td>
<td>2.405</td>
<td>20.29</td>
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<td>10</td>
<td>2.464</td>
<td>30.3</td>
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<td>14.1</td>
<td>2.38</td>
<td>40.4</td>
</tr>
<tr>
<td>18.7</td>
<td>2.41</td>
<td>50.28</td>
</tr>
<tr>
<td>24.8</td>
<td>2.32</td>
<td></td>
</tr>
</tbody>
</table>

enthalpy change

\[ \Delta H/(kJ mol^{-1}) = -1.0 \]

(–16 to 13.9)

#### FIGURE 3.1.1.2.4
Logarithm of K_{OW} and K_{OA} 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: C₈H₁₀, C₂H₅C₆H₅
Molecular Weight: 106.165
Melting Point (°C): –94.96 (Lide 2003)
Boiling Point (°C): 136.2 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C): 0.867 (Weast 1982–83)
Molar Volume (cm³/mol):
  122.4 (20°C, calculated-density, McAuliffe 1966; Stephenson & Malanowski 1987)
  140.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  42.25, 35.2 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion ΔHₕυ (kJ/mol):
  9.184 (Riddick et al. 1986)
  9.16 (Chickos et al. 1999)
Entropy of Fusion ΔSₕυ (J/mol K):
  51.43, 52.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):
140 (15°C, 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°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)
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 (10, 20°C, shake flask-UV, Ben-Naim & Wiff 1979)
181* (vapor saturation-UV, measured range 15–45°C, Sanemasa et al. 1981)
169* (vapor saturation-UV, measured range 15–45°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 γ_w, Hafkenscheid & Tomlinson 1983a)
187 (generator column-HPLC/UV, Wasik et al. 1983)
172 (vapor saturation-UV, Sanemasa et al. 1984)
ln \(x\) = 11.59 – 20.52·\((T_r/K)^{–1}\) + 4.750·\((T_r/K)^{–2}\); \(T_r = T/T_c\), the reduced temp, system temp \(T\) divided by critical temp \(T_c\), temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994c)

ln \(x\) = –30.799 + 3986.26/(T/K) + 7.9095 × 10^{–5}·(T/K)^{2}; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°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* (0°C, mercury manometer, measured range –11.6 to 0°C, Linder 1931)

1546* (30°C, Hg manometer, measured range 10–50°C, Rintelen 1937)

log (P/mmHg) = 22.90283 – 2847.75/(T/K) – 5·log (T/K); temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)

6277* (56.589°C, ebulliometry, measured range 56.589–137.124°C, Willingham et al. 1945)

log (P/mmHg) = 6.94998 – 1419.315/(212.611 + t/°C); temp range 56.6–137.1°C (manometer, Antoine eq. from expit. data, Willingham et al. 1945)

1333* (25.9°C, summary of literature data, Stull 1947)

8399* (63.3°C, static-Hg manometer, measured range 63.3–135.9°C, Buck et al. 1949)

6398* (56.689°C, ebulliometry, measured range 56.689–137.16°C, Forziati et al. 1949)

log (P/mmHg) = 6.95904 – 1425.464/(213.345 + t/°C); temp range 56.7–137.2°C (manometer, Antoine eq. from expit. data, Forziati et al. 1949)

log (P/mmHg) = –3225/(T/K) – 7.553·log (T/K) + 30.49; temp range 80–120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)

1276 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.95719 – 1424.255/(213.206 + t/°C), temp range: 45–190°C (Antoine eq. for liquid state, Dreisbach 1955)

133800* (146.85°C, comparative ebulliometry, measured range 146.85–326.85°C, Ambrose et al. 1967)

log (P/mmHg) = 6.95719 – 1424.255/(213.206 + t/°C); temp range 25.88–163.47°C (Antoine eq. eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 9303.3/(T/K)] + 7.809470; temp range –9.8 to 326.5°C, (Antoine eq., Weast 1972–73)


log (P/atm) = (1 – 409.229/T) × 10^{(0.859833 – 6.85948 × 10^{–5}·T + 5.94439 × 10^{–7}·T^2)}; \(T\) in K, temp range 243.2–615.0 K (Cox vapor pressure eq., Chao et al. 1983)

7120, 1265 (extrapolated-Antoine eq., Boublík et al. 1984; quoted, Howard 1989)

log (P/kPa) = 6.08206 – 1425.305/(213.415 + t/°C), temp range: 25.88–92.7°C (Antoine eq. from reported expit. data, Boublík et al. 1984)

log (P/kPa) = 6.0785 – 1421.653/(212.816 + t/°C); temp range 56.6–137.12°C (Antoine eq. from reported expit. data of Willingham et al. 1945, Boublík et al. 1984)

1268 (interpolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.95719 – 1424.255/(213.21 + t/°C); temp range 26–164°C (Antoine eq., Dean 1985, 1992)

1300 (selected value., Riddick et al. 1986)

log (P/kPa) = 6.09280 – 1431.71/(214.099 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

1266 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 6.06991 – 1416.922/(–69.716 + T/K); temp range 298–420 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.10898 – 1445.262/(–57.128 + T/K); temp range 409–459 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
log \( (P_r/kPa) = 6.36665 - 1665.991/(–26.716 + T/K) \); temp range 457–554 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

log \( (P_r/kPa) = 7.49119 – 3056.747/(159.496 + T/K) \); temp range 549–617 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

1280, 283 (quoted, calculated-UNIFAC activity coeff., Banerjee et al. 1990)

log \( (P/mmHg) = 36.1998 – 3.3402 \times 10^3/(T/K) – 9.7970 \cdot \log (T/K) – 1.1467 \cdot 10^{-11} \cdot (T/K)^2, \) temp range 178–617 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°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* (20.06°C, headspace-GC, Brown & Wasik 1974)
757 (calculated-bond contribution, Hine & Mookerjee 1975)
879 (calculated as \( 1/K_{AW}, C_w/C_A \), reported as expl., 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 \[ \frac{[H/(atm·m³/mol)]}{(T/K)} \] = 11.92 – 4994/(T/K), temp range 10–30°C, EPICS measurements, Ashworth et al. 1988


ln \( K_{AW} = -4567/(T/K) + 0.01047 \cdot Z + 14.001 \); with Z salinity 0–35.5‰, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)

602 (20°C, 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 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log \( K_{AW} = 6.541 – 2100/(T/K) \) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

1173–1273 (27°C, equilibrium headspace-GC, solute concn 0.43–18.66 mg/L, measured range 300–315 K, Cheng et al. 2003)

Octanol/Water Partition Coefficient, \( \log K_{OW} \) at 25°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 & Eganhous 1988)
3.15 (recommended, Sangster 1989, 1993)
3.15 (recommended, Hansch et al. 1995)
3.32, 3.32, 3.53, 3.51 (HPLC-k’ correlation, different combinations of stationary and mobile phases under isotropic conditions, Makovsakya et al. 1995)
3.05 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated
3.85, 3.62, 3.41, 3.24 (20.29, 30.3, 40.4, 50.28°C, from GC-determined $\gamma^\infty$ 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, Abrahm 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-$K_{OW}$, 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 $K_{OC}$ at 25°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 B$_t$ 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 B$_t$ 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-$k'$ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
2.32 (HPLC-screening method, Müller & Körpel 1996)
2.49, 2.73, 2.65, 2.73, 2.77, 2.73 2.74 (2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon $f_{OC} = 4.12$, EPICS-GC/FID, Dewulf et al. 1999)
2.04, 2.18, 1.90 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)

Sorption Partition Coefficient, log $K_{OM}$:
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 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)

Environmental Fate Rate Constants, k, or Half-lives, $t_{1/2}$:
Volatilization: rate constants: $k = 0.035$ d$^{-1}$ with $t_{1/2}$ = 20 d in spring at 8–16°C, $k = 0.331$ d$^{-1}$ with $t_{1/2}$ = 2.1 d in summer at 20–22°C, $k = 0.054$ d$^{-1}$ with $t_{1/2}$ = 13 d in winter at 3–7°C for the periods when volatilization
Mononuclear Aromatic Hydrocarbons

appears to dominate, and \( k = 0.097 \text{ d}^{-1} \) with \( t_{1/2} = 7.1 \text{ d} \) with HgCl\(_2\) in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983);

\( t_{1/2} \) ~ 3.1 h of evaporation from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s at 20°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, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with O\(_3\) or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

\[ k_{\text{OH}} = (4.8 \pm 1.0) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at } 305 \pm 2 \text{ K} \text{ (relative rate method, Lloyd et al. 1976)} \]

\[ k_{\text{OH}} = 4.8 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with } t_{1/2} = 0.24–24 \text{ h} \text{ (Darnall et al. 1976)} \]

\[ k_{\text{OH}} = 15 \text{ h in water, probably not important as aquatic fate (Callahan et al. 1979)} \]

\[ k_{\text{OH}} = 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and residence time of } 1.4 \text{ d, loss of } 51\% \text{ in one day or 12 sunlit hours at } 300 \text{ K in urban environments (Singh et al. 1981)} \]

\( k << 360 \text{ M}^{-1} \text{ h}^{-1} \) for singlet oxygen and 720 M\(^{-1}\) h\(^{-1}\) for RO\(_2\) radical (Mabey et al. 1982)

\[ k_{\text{OH}} = 4.4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \text{ with } t_{1/2} = 1.3 \text{ d in the atmosphere (Mill 1982)} \]

\[ k_{\text{O}_3} = 340 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ at } 300 \text{ K (Lyman et al. 1982)} \]

\[ k = (14 \pm 4) \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone in water using } 100 \text{ mM } \text{t-BuOH as scavenger at } pH 2.0 \text{ and } 20–23°C \text{ (Hoigné & Bader 1983)} \]

Hydrolysis: not aquatically significant (Callahan et al. 1979);

no hydrolyzable functional groups (Mabey et al. 1982)

Biodegradation:

\[ 100\% \text{ biodegraded after } 192 \text{ h at } 13°C \text{ with an initial concn of } 1.36 \times 10^{-6} \text{ L/L (Jamison et al. 1976)} \]

\[ t_{1/2(aq. \text{ aerobic})} = 72–240 \text{ h, based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991)} \]

\[ t_{1/2(aq. \text{ anaerobic})} = 4224–5472 \text{ h, based on anaerobic groundwater die-away test data (Wilson et al. 1986; Howard et al. 1991)} \]

\[ k = 0.5 \text{ d}^{-1}, \text{ significant degradation under favourable conditions in an aerobic environment (Tabak et al. 1981; Mills et al. 1982)} \]

\[ t_{1/2} \sim 2 \text{ d degradation by established microorganisms depending on body of water and its temperature (Howard 1989)} \]

\[ k = 0.07 \text{ yr}^{-1} \text{ with } t_{1/2} = 37 \text{ d (Olsen & Davis 1990)} \]

Biotransformation: \( 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1} \) (Mabey et al. 1982).

Half-Lives in the Environment:

Air: \( t_{1/2} = 0.24–24 \text{ h}, \text{ based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976)} \);

photodecomposition \( t_{1/2} = 5.0 \text{ h} \text{ under simulated atmospheric conditions, with NO (Dilling et al. 1976)} \);

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 \( \tau = 20 \text{ h} \text{ due to reaction with OH radical (Altshuller 1991)} \);

\[ t_{1/2} = 8.56–85.6 \text{ h (Atkinson 1985)} \]

\( t_{1/2} = 6.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (relative rate method, Ohta & Ohyama 1985)} \]

\[ k_{\text{OH}}(\text{calc}) = 6.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR [structure-activity relationship], Atkinson 1987)} \]

\[ k_{\text{OH}} = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } -298 \text{ K (recommended, Atkinson 1989, 1990)} \]

\[ k_{\text{OH}}(\text{calc}) = 6.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)} \]

Surface Water: \( t_{1/2} = 5–6 \text{ h (Callahan et al. 1979)} \), based on the estimated evaporative loss of toluene at 25°C and 1 m depth of water (Mackay & Leinonen 1975)

\[ t_{1/2} = 20 \text{ d in spring at } 6–16°C, t_{1/2} = 2.1 \text{ d in summer at } 20–22°C, t_{1/2} = 13 \text{ d in winter at } 3–7°C \text{ and } t_{1/2} = 7.1 \text{ d with HgCl}_2 \text{ in marine mesocosm experiments (Wakeham et al. 1983)} \]

\[ t_{1/2} = 72–240 \text{ h, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991)} \]

Surface Water: \( t_{1/2} = 5–6 \text{ h (Callahan et al. 1979)} \), based on the estimated evaporative loss of toluene at 25°C and 1 m depth of water (Mackay & Leinonen 1975)

Ground water: \( t_{1/2} = 144–5472 \text{ h, based on unacclimated aqueous aerobic biodegradation half-life and seawater dieaway test data (Van der Linden 1978; Howard et al. 1991)} \)

\( t_{1/2} \sim 0.3 \text{ yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981)} \).
Soil: $t_{1/2} = 72–240$ h, based on unacclimated aqueous aerobic biodegradation half-life (Van der Linden 1978; Howard et al. 1991); $t_{1/2} < 10$ d (Ryan et al. 1988).

### Biota:

**TABLE 3.1.1.3.1**

Reported aqueous solubilities of ethylbenzene at various temperatures


<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>S/g·m$^{-3}$</th>
<th>$t/°C$</th>
<th>S/g·m$^{-3}$</th>
<th>$t/°C$</th>
<th>S/g·m$^{-3}$</th>
<th>$t/°C$</th>
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<td>192</td>
<td>20</td>
<td>212</td>
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<tr>
<td>20.7</td>
<td>207</td>
<td>7.1</td>
<td>186</td>
<td>9</td>
<td>187</td>
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<td>11.8</td>
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$\Delta H_{\text{sol}}$(kJ mol$^{-1}$) =

- 25°C: 1.6
- 2°C: -3.98
- 7°C: -2.74
- 12°C: -1.63
- 17°C: -0.343
- 22°C: -0.167
- 27°C: 1.97
- 32°C: 3.615
- 37°C: 7.36


<table>
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<th>$t/°C$</th>
<th>S/g·m$^{-3}$</th>
<th>$t/°C$</th>
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$\Delta H_{\text{sol}}$(kJ mol$^{-1}$) = 3.60

at 25°C

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$\Delta H_{\text{sol}}$(kJ mol$^{-1}$) = 2.1
TABLE 3.1.1.3.1 (Continued)

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<td>S/g·m⁻³</td>
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*ΔHᵣₒ(l/kJ mol⁻¹) = 3.90 at 25°C*

<table>
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<th>Dohányosová et al. 2001</th>
<th>Sawamura et al. 2001</th>
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*ΔHᵣₒ(l/kJ mol⁻¹) = 3.0 at 25°C*

**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

<table>
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<tr>
<th>Equation</th>
<th>Description</th>
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<tr>
<td>( \log P = A - \frac{B}{T/K} )</td>
<td>(1) ( \log P = A - \frac{B}{C + T/K} )</td>
</tr>
<tr>
<td>( \ln P = A - \frac{B}{T/K} )</td>
<td>(1a) ( \ln P = A - \frac{B}{C + T/K} )</td>
</tr>
<tr>
<td>( \log P = A - \frac{B}{C + \frac{t}{°C}} )</td>
<td>(2) ( \log P = A - \frac{B}{C + \frac{t}{°C}} )</td>
</tr>
<tr>
<td>( \log P = A - \frac{B}{C + T/K} - C \log (T/K) )</td>
<td>(3)</td>
</tr>
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</table>

1. **Linder 1931**

<table>
<thead>
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<th>Temperature (°C)</th>
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<td>–1.20</td>
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</table>

**Willingham et al. 1945**

<table>
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<td>–9.8</td>
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<tr>
<td>–9.8</td>
<td>1013</td>
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<tr>
<td>6.7</td>
<td>1013</td>
</tr>
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</table>

**Stull 1947**

**Buck et al. 1949**

<table>
<thead>
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<th>Temperature (°C)</th>
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<tbody>
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2. **Forziati et al. 1949**

<table>
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<th>Vapor Pressure (Pa)</th>
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<td>56.689</td>
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<tr>
<td>60.887</td>
<td>7690</td>
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<td>64.51</td>
<td>8990</td>
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**Ambrose et al. 1967**

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**Zwolinski & Wilhoit 1971**

<table>
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**Osborn & Scott 1980**

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### TABLE 3.1.1.3.2 (Continued)

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<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
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<td>P/Pa</td>
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**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

\[
\ln K_{AW} = A - B/(T/K) \quad (1)
\]

\[
\ln (1/K_{AW}) = A - B/(T/K) \quad (2)
\]

\[
\ln [H/(Pa m^3/mol)] = A - B/(T/K) \quad (3)
\]

\[
K_{AW} = A - B/(T/K) + C\cdot(T/K)^2 \quad (5)
\]

#### 1.

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<td>vapor-liquid equilibrium</td>
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<td>H/(Pa m^3/mol)</td>
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#### 2.

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<td>H/(Pa m^3/mol)</td>
<td>H/(Pa m^3/mol)</td>
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**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: \( C_8H_{10} \), \( C_6H_4(CH_3)_2 \)
Molecular Weight: 106.165
Melting Point (°C):
\(-25.2\)  \( \) (Weast 1982–83; Lide 2003)
Boiling Point (°C):
144.5  \( \) (Lide 2003)
Density (g/cm\(^3\) at 20°C):
0.8802  \( \) (Weast 1982–83)
Molar Volume (cm\(^3\)/mol):
120.6  \( \) (20°C, calculated-density)
140.4  \( \) (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
43.434, 36.82  \( \) (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion \( \Delta H_{m\text{fus}} \) (kJ/mol):
13.6  \( \) (Chickos et al. 1999)
Entropy of Fusion \( \Delta S_{m\text{fus}} \) (J/mol K):
55.23  \( \) (Yalkowsky & Valvani 1980)
54.9, 45.5  \( \) (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°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°C, shake flask-UV, Ben-Naim & Wiff 1979)
179*  \( \) (vapor saturation-UV spec., measured range 15–45°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°C, Shaw 1989b)

Vapor Pressure (Pa at 25°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*  \( \) (0.60°C, mercury manometer, measured range –17 to 0.60°C, Linder 1931)
767*  \( \) (20°C, Hg manometer, Kassel 1936)
\[ \log (P/mmHg) = -2830.0/(T/K) – 5·\log (T/K) + 22.7480; \] temp range 0–80°C (vapor pressure eq. from Hg manometer measurements, Kassel 1936)
987*  \( \) (30°C, Hg manometer, measured range 10–50°C, Rintelen et al. 1937)
log (P/mmHg) = –2908.07/(T/K) – 5·log (T/K) + 22.95279; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)

880* (Hg manometer measurements, Pitzer & Scott 1943)

log (P/mmHg) = –3327.16/(T/K) – 8.0 log (T/K) + 31.7771 ; temp range 0–60°C (manometer, three-constant vapor pressure eq. from exp. data, Pitzer & Scott 1943)

6354* (63.46°C, ebulliometry, measured range 63.46–145.36°C, Willingham et al. 1945)

6401* (63.608°C, ebulliometry, measured range 63.608–145.400°C, Forziati et al. 1949)

log (P/mmHg) = 6.99937 – 1474.969/(213.714 + t/°C); temp range 63.5–145.4°C (manometer, Antoine eq. from exp. data, Willingham et al. 1945)

266.6* (20.2°C, summary of literature data, Stull 1947)

log (P/mmHg) = 6.99891 – 1474.679/(213.686 + t/°C); temp range 63.6–145.4°C (manometer, Antoine eq. from exp. data, Forziati et al. 1949)

1333* (32.155°C, compiled data, temp range 32.155–172.095°C, Bond & Thodos 1960)

108000* (146.85°C, ebulliometry, measured range 146.85–346.85°C, Ambrose et al. 1967)

882* (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.99891 – 1474.679/(213.686 + t/°C); temp range 32.14–172.07°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = –0.2185 × 9998.5/(T/K) + 8.147551; temp range –3.8 to 144.4°C (Antoine eq., Weast 1972–73)

log (P/atm) = (1 – 417.496/T) × 10^(0.855257 – 6.48662 × 10^(-4·T) + 5.53883 × 10^7·T^2); 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 (P/kPa) = 6.12699 – 1476.753/(213.911 + t/°C); temp range 63.46–145.4°C (Antoine eq. from reported exp. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 5.9422 – 1387.336/(206.409 + t/°C); temp range 0–50°C (Antoine eq. from reported exp. data of Pitzer & Scott 1943, Boublik et al. 1984)

882 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 6.99891 – 1474.679/(213.69 + t/°C); temp range 32–172°C (Antoine eq., Dean 1985, 1992)

880 (Riddick et al. 1986)

log (P/kPa) = 6.13072 – 1479.82/(214.315 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

885 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 6.13132 – 1480.155/(–58.804 + T/K); temp range 333–419 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.15921 – 1502.949/(–55.725 + T/K); temp range 416–471 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.46119 – 1772.963/(–18.84 + T/K); temp range 471–571 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)

log (P/kPa) = 7.91427 – 3735.582/(229.953 + T/K); temp range 567–630 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P/mmHg) = 37.2413 – 3.4573 × 10^3/(T/K) – 10.126·log (T/K) + 9.0676 × 10–11·(T/K)^2, temp range 248–630 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°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/K_{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 (20°C, EPICS-GC, Yurteri et al. 1987)

493* (EPICS-GC/FID, Ashworth et al. 1988)

ln [H/(atm·m³/mol)] = 5.541 – 3220/(T/K); temp range 10–30°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°C, equilibrium headspace-GC, Kolb et al. 1992)
\ln \left( \frac{1}{K_{AW}} \right) = -7.61 + \frac{2647}{(T/K)}, \ \text{temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)}

- 485\* \quad \text{(infinite activity coeff. \(\gamma^-\) in water determined by inert gas stripping-GC, Li et al. 1993)}
- 506 \* \quad \text{(static headspace-GC, Robbins et al. 1993)}
- 372 \quad \text{(headspace solid-phase microextraction (SPME)-GC, Zhang & Pawliszyn 1993)}
- 429 \* \quad \text{(EPICS-GC/FID, measured range 2–25°C, Dewulf et al. 1995)}
- 189, 496 \quad \text{(6.0, 25°C, EPICS-GC/FID, natural seawater with salinity of 35‰, Dewulf et al. 1995)}

\ln K_{AW} = -4232/(T/K) + 0.01115\cdot Z + 12.400; \ \text{with } Z \text{ salinity 0–35.5%, temp range: 2–35°C (EPICS-GC/FID, Dewulf et al. 1995)}

\log K_{AW} = 5.064 – 1719/(T/K) \quad \text{(van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)}

Octanol/Water Partition Coefficient, \log K_{ow} at 25°C:

\begin{align*}
3.15 & \quad \text{(calculated-\(\pi\) substituent constant, Hansch et al. 1968)} \\
2.73 & \quad \text{(shake flask-LSC, Banerjee et al. 1980)} \\
3.19 & \quad \text{(HPLC-k’ correlation, Hammers et al. 1982)} \\
3.13 & \quad \text{(generator column-HPLC/UV, Tewari et al. 1982b,c)} \\
3.13 & \quad \text{(generator column-HPLC/UV, Wasik et al. 1983)} \\
3.13, 3.14, 3.06, 3.16, 3.42 & \quad \text{(quoted exptl.; calculated-\(\pi\) const., f const., MW, MCI \(\chi\), TSA, Doucette & Andren 1988)} \\
3.25, 3.35 & \quad \text{(RP-HPLC-k’ capacity factor correlations, Sherblom & Eganhouse 1988)} \\
3.12 & \quad \text{(recommended, Sangster 1989)} \\
3.18 & \quad \text{(normal phase HPLC-k’ correlation, Govers & Evers 1992)} \\
3.12 & \quad \text{(recommended, Hansch et al. 1995)} \\
\end{align*}

Octanol/Air Partition Coefficient, \log K_{oa} at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

\begin{align*}
3.80^* & \quad \text{(30.3°C, from GC-determined \(\gamma^-\) in octanol, measured range 30.3–50.28°C, Gruber et al. 1997)} \\
3.72 & \quad \text{(calculated-measured \(\gamma^-\) in pure octanol of Tewari et al. 1982, Abraham et al. 2001)} \\
\end{align*}

Bioconcentration Factor, log BCF:

\begin{align*}
1.33 & \quad \text{(eels, Ogata & Miyake 1978)} \\
0.79 & \quad \text{(clams, Nunes & Benville 1979)} \\
1.15 & \quad \text{(goldfish, Ogata et al. 1984)} \\
2.34 & \quad \text{((S. capricornutum, Herman et al. 1991)} \\
\end{align*}

Sorption Partition Coefficient, \log K_{oc} at 25°C:

\begin{align*}
1.68–1.83 & \quad \text{(Nathwani & Philip 1977)} \\
2.35 & \quad \text{(sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)} \\
2.73 & \quad \text{(HPLC-k’ correlation, cyanopropyl column, Hodson & Williams 1988)} \\
2.37, 2.40 & \quad \text{(RP-HPLC-k’ correlation, cyanopropyl column, Szabo et al. 1990a,b)} \\
3.13 & \quad \text{(average of 5 soils, sorption isotherms by batch equilibrium method, Xing et al. 1994)} \\
2.36, 2.65, 2.65 & \quad \text{(RP-HPLC-k’ correlation on 3 different stationary phases, Szabo et al. 1995)} \\
2.45, 2.45 & \quad \text{(RP-HPLC-k’ 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 \text{(2.3, 3.8, 6.2, 8.0, 13.5, 18.6, 25°C, natural sediment from River Leie, organic carbon } f_{oc} = 4.12\%, \text{ EPICS-GC/FID, Dewulf et al. 1999)} \\
\end{align*}

Environmental Fate Rate Constants, k, or Half-Lives, \(t_{\text{1/2}}\):

- Volatilization: \(t_{\text{1/2}} = 5.61 \text{ h from water depth of 1 m (Mackay & Leinonen 1975; Haque et al. 1980)}\)
- \(t_{\text{1/2}} \sim 3.2 \text{ h of evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s (Lyman et al. 1982)}\)
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$\tau_0 \sim 31–125$ h of evaporation from a typical river or pond (Howard 1990).

Photolysis: $k = 7.46 \times 10^{-3}$ h$^{-1}$ with H$_2$O$_2$ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant $k$; for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated $^*$, see reference:

$k_{OH} = (7.7 \pm 2.3) \times 10^6$ L mol$^{-1}$ s$^{-1}$; $k_{O_3P} = (1.05 \pm 0.11) \times 10^6$ L mol$^{-1}$ s$^{-1}$ with O($^3$P) atom at room temp.

(relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (15.3 \pm 1.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{O_3P} = (1.74 \pm 0.18) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction of O($^3$P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 8.4 \times 10^6$ L mol$^{-1}$ s$^{-1}$ with $\tau_0 = 0.24–24$ h (Darnall et al. 1976)

$k_{OH}^* = (14.3 \pm 1.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = (12.9, 13.0, 12.4) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)

$k_{OH} = 13.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ 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)

$k_{O_3} \leq 0.01 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 ± 2 K with a calculated lifetime $\tau > 2300$ d, and a calculated lifetime of 0.8 d due to reaction with OH radical at room temp. (Atkinson et al. 1982)

$k_{O_3} = 950$ cm$^3$ mol$^{-1}$ s$^{-1}$ at 300 K (Lyman et al. 1982)

$k_{OH} = (5.9–12) \times 10^9$ M$^{-1}$ s$^{-1}$ with $\tau_0 = 0.47–1.0$ d (Mill 1982)

$k = (90 \pm 20)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 1.7–5.0 and 20–23°C (Hoigné & Bader 1983)

$k_{O_3} = 1.1 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{OH} = 13.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with $\tau_0 = 4.4–44$ h (Atkinson 1985)

$k_{OH} = 12.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (relative rate method, Ohta & Ohyama 1985)

$k_{OH} = 12.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 24.2°C, with a calculated atmospheric lifetime of 0.93 d (Edney et al. 1986)

$k_{OH}(calc) = 6.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = 14.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR [structure-activity relationship] Atkinson 1987)

$k_{OH} = 1.47 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO_3} = 3.74 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{O_3} = 0.01 \times 10^{-18}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH} = 1.47 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{NO_3} = 3.7 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson & Aschmann 1988)

$k_{OH}^* = 1.37 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ independent over 296–320 K (recommended, Atkinson 1989)

$k_{OH} = 13.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1990)

$k_{OH}(calc) = 6.92 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH}(calc) = 14.75 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klant 1993)

$k_{OH}(calc) = 6.51 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(exptl) = 13.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ 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°C with an initial concn of 1.62 \times 10^{-6} L/L (Jamison et al. 1976);

$\tau_{50}(aq. Aerobic) = 168–672$ 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)

$\tau_{50}(aq. anaerobic) = 4320–8640$ 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 aerobic river/groundwater infiltration system (Kuhn et al. 1985; Howard et al. 1991)

$k = 0.06$ yr$^{-1}$ with $\tau_0 = 32$ d (Olsen & Davis 1990)

$\tau_{50}(aerobic) = 7$ d, $\tau_{50}(anaerobic) = 180$ d in natural waters (Capel & Larson 1995)

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $\tau_0 = 0.24–2.4$ h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976);
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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 $\tau > 2300$ d and 0.8 d due to reactions with $O_3$ and OH radical respectively at room temp.
(Atkinson et al. 1982);
$\tau_{s} = 4.4-44$ h, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);
summer daylight lifetime $\tau = 10$ 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 $\tau_s = 3.9 \times 10^5 - 2.7 \times 10^8$ h in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974);
$\tau_{s} = 5.18$ h, based on evaporative loss at 25°C and 1 m depth of water (Mackay & Leinonen 1975; Haque et al. 1980);
$\tau_{s} = 168-672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);
$\tau_{s} = 1-5$ d, volatilization to be the dominant removal process (Howard 1990).
$\tau_{s}$(aerobic) = 7 d, $\tau_{s}$(anaerobic) = 180 d in natural waters (Capel & Larson 1995).
Ground water: $\tau_s = 336-8640$ 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);
$\tau_{s} \approx 0.3$ yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981).
Soil: $\tau_{s} = 168-672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).
Biota: $\tau_{s} = 2$ 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

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</table>

| 45         | 210             |                     | 45             |                     |

**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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) + D \cdot P/(T/K)^2
\end{align*}
\]

1. **Kassel 1936**

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<td>3680</td>
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<td>144.0–144.1°C</td>
</tr>
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<td>70</td>
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<td>b.p. 144.0–144.1°C</td>
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<tr>
<td>80</td>
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<td>–17 26.66</td>
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2. **Rintelen et al. 1937**

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3. **Stuckey & Saylor 1940**

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4. **Pitzer & Scott 1943**

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5. **Linder 1931**

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6. **Willingham et al. 1945**

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7. **Stull 1947**

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8. **Forziati et al. 1949**

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9. **Bond & Thodos 1960**

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\[ \Delta H_v/(kJ \text{ mol}^{-1}) = 43.806 \text{ at } 25°C \]
### TABLE 3.1.1.4.2 (Continued)

<table>
<thead>
<tr>
<th>Willingham et al. 1945</th>
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<th>Forziati et al. 1949</th>
<th>Bond &amp; Thodos 1960</th>
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<td>ebulliometry</td>
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<td>1474.679</td>
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<td>bp/°C</td>
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3.

<table>
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<th>Ambrose et al. 1967</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
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<tr>
<td>D</td>
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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

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<td>t/°C</td>
<td>H/(Pa m³/mol)</td>
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A 5.541 B 2647/R A 17.67818 B 4243
B 3220 B 3397.97

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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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<td>50.28</td>
<td>3.38</td>
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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: C₈H₁₀, C₆H₄(CH₃)₂  
Molecular Weight: 106.165  
Melting Point (°C):  
–47.8  (Lide 2003)  
Boiling Point (°C):  
139.12  (Lide 2003)  
Density (g/cm³ at 20°C):  
0.8842  (Weast 1982–83)  
Molar Volume (cm³/mol):  
120.1  (20°C, calculated-density)  
140.4  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):  
42.656, 36.36  (25°C, bp, Riddick et al. 1986)  
Enthalpy of Fusion ΔHₒ (kJ/mol):  
11.57  (Chickos et al. 1999)  
Entropy of Fusion ΔSₒ (J/mol K):  
51.88  (Yalkowsky & Valvani 1980)  
51.4, 45.6  (exptl., calculated-group additivity method, Chickos et al. 1999)  
Fugacity Ratio at 25°C, F: 1.0  

Water Solubility (g/m³ or mg/L at 25°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°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°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°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°C, Shaw 1989b)  

Vapor Pressure (Pa at 25°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*  (–2.8°C, mercury manometer, measured range –8.40 to –2.8°C, Linder 1931)  
833*  (20°C, Hg manometer, Kassel 1936)  
log (P/mmHg) = –2876.3/(T/K) – 5·log (T/K) + 22.9425; temp range 0–80°C (vapor pressure eq. from Hg manometer measurements, Kassel 1936)  
1213*  (30°C, Hg manometer, measured range 10–50°C, Rintelen et al. 1937)
log (P/mmHg) = –2870.38/(T/K) – 5·log (T/K) + 22.92341; temp range 4–75°C (vapor pressure eq. from manometer measurements, Stuckey & Saylor 1940)

1113* (Hg manometer, measured range 0–60°C, Pitzer & Scott 1943)
log (P/mmHg) = –2871.66/(T/K) – 5·log (T/K) + 22.9270; temp range 0–60°C (manometer, three-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)

6355* (59.203°C, ebulliometry, measured range 59.203–140.041°C, Willingham et al. 1945)
log (P/mmHg) = 7.00343 – 1458.214/(214.609 + t/°C); temp range 59.2–140.0°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

266.6* (16.8°C, summary of literature data, temp range –6.9 to 139.1°C, Stull 1947)

6400* (59.335°C, ebulliometry, measured range 59.335–140.078°C, Forziati et al. 1949)
log (P/mmHg) = 8.00849 – 1461.925/(215.073 + t/°C); temp range 59.3–140.1°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

1115 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.00908 – 1462.266/(215.105 + t/°C); temp range 45–195°C (Antoine eq. for liquid state, Dreisbach 1955)

124200* (146.85°C, ebulliometry, measured range 146.85–316.85°C, Ambrose et al. 1967)
log (P/mmHg) = 6.4729 – 1640.82/(230.899 + t/°C); temp range 0–60°C (Antoine eq. from reported exptl. data of Pitzer & Scott 1943, Boublik et al. 1984)

1106 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.00908 – 1462.266/(215.11 + t/°C); temp range 28–166°C (Antoine eq., Dean 1985, 1992)

1100* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.00908 – 1462.266/(215.105 + t/°C); temp range 28.24–166.39°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 9904.2/(T/K)] + 8.167049; temp range –6.9 to 139.1°C (Antoine eq., Weast 1972–73)

log (P/atm) = (1 – 3412.335/T) × 10^(0.859841 – 6.73249 × 10^4·T + 5.87438 × 10^7·T^2); 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 (P/kPa) = 6.47232 – 1460.805/(214.895 + t/°C); temp range 0–60°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 7.00908 – 1462.266/(215.105 + t/°C); temp range 28.24–166.39°C (Antoine eq. from reported exptl. data of Willingham et al. 1945, Boublik et al. 1984)

log (P/kPa) = 6.4729 – 1641.628/(230.899 + t/°C); temp range: 0–60°C (Antoine eq. from reported exptl. data of Pitzer & Scott 1943, Boublik et al. 1984)

log (P/kPa) = 6.13785 – 1465.39/(215.512 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

1110 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P L/kPa) = 6.14083 – 1457.244/(–57.442 + T/K); temp range 331–414 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P L/kPa) = 5.76037 – 1292.22/(–72.052 + T/K); temp range 267–301 K (Antoine eq.-II, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.17035 – 1490.184/(–54.184 + T/K); temp range 412–554 K (Antoine eq.-III, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.42535 – 1710.901/(–24.591 + T/K); temp range 461–554 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P L/kPa) = 7.59221 – 3165.34/(165.278 + T/K); temp range 550–617 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P L/kPa) = 6.42535 – 1710.901/(–24.591 + T/K); temp range 461–554 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

log (P L/kPa) = 7.59221 – 3165.34/(165.278 + T/K); temp range 550–617 K (Antoine eq.-V, Stephenson & Malanowski 1987)

log (P L/kPa) = 34.6809 – 3.2981 × 10^4/(T/K) – 9.2570 × 10^-10·(T/K) + 2.4103 × 10^-6·(T/K)^2, temp range 226–617 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°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 [H/(atm·m³/mol)] = 6.280 – 3337/(T/K); temp range: 10–30°C (EPICS measurements, Ashworth et al. 1988)
675 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
665 (infinite activity coeff. γ∞ 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°C, Dewulf et al. 1995)
Mononuclear Aromatic Hydrocarbons

\[ \ln K_{AW} = -4026/(T/K) + 0.00846 \cdot Z + 12.123; \text{ with } Z \text{ salinity } 0-35.5\%, \text{ temp range: } 2-35°C \text{ (EPICS-GC/FID, Dewulf et al. 1995)} \]

590 \hspace{1cm} (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

658.5 \hspace{1cm} (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

561 \hspace{1cm} (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

\[ \log K_{AW} = 5.204 - 1713/(T/K) \text{ (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)} \]

Octanol/Water Partition Coefficient, \( \log K_{OW} \) at 25°C:

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<tr>
<th>Value</th>
<th>Source</th>
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<td>HPLC-k’ correlation, Hammers et al. 1982</td>
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<td>generator column-HPLC/UV, Tewari et al. 1982b,c</td>
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<tr>
<td>3.20</td>
<td>generator column-HPLC/UV, Wasik et al. 1983</td>
</tr>
<tr>
<td>3.28</td>
<td>HPLC-RV retention volume correlation, Garst &amp; Wilson 1984</td>
</tr>
<tr>
<td>3.37</td>
<td>HPLC-k’ correlation, Haky &amp; Young 1984</td>
</tr>
<tr>
<td>3.33, 3.45</td>
<td>RP-HPLC-k’ capacity factor correlations, Sherblom &amp; Eganhouse 1988</td>
</tr>
<tr>
<td>3.20</td>
<td>(recommended, Sangster 1989, 1993)</td>
</tr>
<tr>
<td>3.31</td>
<td>(normal phase HPLC-k’ correlation, Gover &amp; Evers 1992)</td>
</tr>
<tr>
<td>3.20</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
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</table>

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.69*</td>
<td>(30.3°C, from GC-determined ( \gamma^\infty ) in octanol, measured range 30.3-50.28°C, Gruber et al. 1997)</td>
</tr>
<tr>
<td>3.79</td>
<td>(calculated-measured ( \gamma^\infty ) in pure octanol of Tewari et al. 1982, Abraham et al. 2001)</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, \( \log BCF \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Species, Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.37</td>
<td>eels, Ogata &amp; Miyake 1978</td>
</tr>
<tr>
<td>0.78</td>
<td>clams, Nunes &amp; Benville 1979</td>
</tr>
<tr>
<td>1.17</td>
<td>goldfish, Ogata et al. 1984</td>
</tr>
<tr>
<td>2.40</td>
<td>( S. \text{ capricornutum} ), Herman et al. 1991</td>
</tr>
</tbody>
</table>

Sorption Partition Coefficient, \( \log K_{OC} \) at 25°C:

<table>
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<tbody>
<tr>
<td>2.11, 2.48, 2.20</td>
<td>(forest soil pH 5.6, forest soil pH 4.2, agricultural soil pH 7.4, Seip et al. 1986)</td>
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<tr>
<td>2.37, 2.40</td>
<td>RP-HPLC-k’ correlation, Szabo et al. 1990a,b</td>
</tr>
<tr>
<td>2.62, 2.63</td>
<td>RP-HPLC-k’ correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996</td>
</tr>
<tr>
<td>2.06, 2.33</td>
<td>(soils: organic carbon OC ( \geq ) 0.1%, OC ( \geq ) 0.5%, average, Delle Site 2001)</td>
</tr>
</tbody>
</table>

Environmental Fate Rate Constants, k, or Half-Lives, \( t_\text{½} \):

Volatilization: \( t_\text{½} \approx 3.1 \text{ h for evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s (Lyman et al. 1982)} \);

\( t_\text{½} \approx 27-135 \text{ h for evaporation from a typical river or pond (Howard 1990)} \).

Photolysis:

Oxidation: rate constant k; for gas-phase second-order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO₃ radical and \( k_{O_3} \) with O₃ or as indicated. Data at other temperatures and/or the Arrhenius expression are designated *, see reference:

photooxidation \( t_\text{½} = 4.8 \times 10^6 \text{-} 2.4 \times 10^8 \text{ h in water, based on estimated rate data for alkoxy radical in aqueous solution (Hendry et al. 1974)} \)

\[ k_{OH} = (14 \pm 1) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with } t_\text{½} = 0.83 \text{ h; } k_{O_3} = (2.12 \pm 0.21) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with O(3P) atom at room temp. (relative rate method, Doyle et al. 1975)} \]

\[ k_{OH} = 1.4 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1} \text{ with an initial concn of } 2.0 \times 10^{-10} \text{ mol L}^{-1} \text{ at 300 K (Doyle et al. 1975)} \]

\[ k_{OH} = (23.6 \pm 2.4) \times 10^{-12} \text{ cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } k_{O_3} = (3.52 \pm 0.35) \times 10^{-13} \text{ cm}^{-3} \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction of O(3P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)} \]

\[ k_{OH} = (12.9 \pm 2.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at 305 \pm 2 K (relative rate method, Lloyd et al. 1976)} \]
\[ k_{\text{OH}} = 14.1 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \] with \( t_{\frac{1}{2}} = 0.24-2.4 \text{ h} \) (Darnall et al. 1976)

\[ k_{\text{OH}}^* = (24.0 \pm 2.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at room temp., measured over temp range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

\[ k_{\text{OH}} = (15.6 - 21.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishanakara et al. 1978)

\[ k_{\text{OH}} = 23.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] 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)

\[ k_{\text{O}_3} = 0.005 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with a calculated lifetime \( \tau > 1150 \text{ d} \) and a lifetime \( \tau = 0.5 \text{ d} \) due to reaction with OH radical at room temp. (Atkinson et al. 1982)

\[ k_{\text{O}_3} = 780 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \] for the reaction with ozone at 300 K (Lyman et al. 1982)

\[ k_{\text{OH}} = (5.9-12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with \( t_{\frac{1}{2}} = 0.47-1.0 \text{ d} \) for xylenes (Hoffman 1982)

\[ k_{\text{NO}_3} = 7.1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 296 K (Atkinson et al. 1984)

\[ k_{\text{OH}} = 23.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (Ohta & Ohyama 1985)

\[ k_{\text{OH}} = 22.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 23.5°C, with a calculated atmospheric lifetime \( \tau = 0.51 \text{ d} \) (Edney et al. 1986)

\[ k_{\text{OH}} = (94 \pm 20) \text{ M}^{-1} \text{ s}^{-1} \] for the reaction with ozone in water using 1 mM t-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

\[ k_{\text{NO}_3} = 2.49 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

\[ k_{\text{NO}_3} = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (recommended, Atkinson 1989, 1990)

\[ k_{\text{OH}} = 2.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

\[ k_{\text{OH}} = 1.45 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (estimated by SARs, Müller & Klein 1992)

\[ k_{\text{OH}} = 17.47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] (molecular orbital calculations, Klamt 1993)

\[ k_{\text{OH}} = (1.81 \pm 0.40) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] and \( (2.03 \pm 0.10) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 ± 2 K (relative rate method. Phousongphouang & Arey 2002)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of \( 3.28 \times 10^{-6} \text{ L/L} \) (Jamison et al. 1976)

\( t_{\frac{1}{2}}(\text{aq. aerobic}) = 168-672 \text{ h} \), 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)

\( t_{\frac{1}{2}}(\text{aq. anaerobic}) = 672-2688 \text{ h} \), based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)

\( t_{\frac{1}{2}} = 0.03 \text{ d} \) (Olsen & Davis 1990)

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: \( t_{\frac{1}{2}} = 0.83 \text{ h} \), based on rate of disappearance for the reaction with OH radical in ambient LA basin air at 300 K (Doyle et al. 1975);

photodecomposition \( t_{\frac{1}{2}} = 2.9 \text{ h} \) under simulated atmospheric conditions, with NO (Dilling et al. 1976);

estimated lifetime \( \tau = 1.5 \text{ h} \) 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 \( \tau > 1150 \text{ d} \) and 0.5 d due to reactions with \( \text{O}_3 \) and OH radical, respectively, at room temp. (Atkinson et al. 1982);

\( t_{\frac{1}{2}} = 2.6-26 \text{ h} \), based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991);

summer daylight lifetime \( \tau = 0.51 \text{ d} \) due to reaction with OH radical (Edney et al. 1986);

summer daylight lifetime \( \tau = 5.9 \text{ h} \) due to reaction with OH radical (Altshuller 1991);

calculated lifetimes of 5.9 h, 200 d and > 4.5 yr for reactions with OH radical, \( \text{NO}_3 \) radical and \( \text{O}_3 \), respectively (Atkinson 2000).

Surface Water: \( t_{\frac{1}{2}} = 168-672 \text{ h} \), 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 \( t_{\frac{1}{2}} = 1-5.5 \text{ d} \) (Howard 1990).
Ground water: $t_\frac{1}{2} = 336–8640$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.60$ at 25°C

Soil: $t_\frac{1}{2} = 168–672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991).

Table 3.1.1.5.1

<table>
<thead>
<tr>
<th>Table 3.1.1.5.1</th>
<th>Reported aqueous solubilities of $m$-xylene at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bohon &amp; Claussen 1951</td>
<td>shake flask-UV</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>S/g·m$^{-3}$</td>
</tr>
<tr>
<td>0.4</td>
<td>209</td>
</tr>
<tr>
<td>5.2</td>
<td>201</td>
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<tr>
<td>14.9</td>
<td>192</td>
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<tr>
<td>21</td>
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<td>25</td>
<td>196</td>
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<td>25.6</td>
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<td>34.9</td>
<td>203</td>
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<tr>
<td>39.6</td>
<td>218</td>
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</table>

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.60$ at 25°C

<table>
<thead>
<tr>
<th>Chernogolazova &amp; Simulin 1976</th>
<th>synthetic method-GC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>S/g·m$^{-3}$</td>
</tr>
<tr>
<td>25°C</td>
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<td>22°C</td>
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<td>27°C</td>
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<tr>
<td>32°C</td>
<td>3.92</td>
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<td>37°C</td>
<td>8.87</td>
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$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 11.9$

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 2.9$

(calc from Van’t Hoff eq.)

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 \textit{m}-xylene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) + D(T/K)^2 \quad (5)
\end{align*}
\]

1.

<table>
<thead>
<tr>
<th>Kassel 1936</th>
<th>Rintelen et al. 1937</th>
<th>Pitzer &amp; Scott 1943</th>
<th>Willingham et al. 1945</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>0</td>
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<td>10</td>
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<td>eq. 4</td>
<td>P/mmHg</td>
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</tr>
<tr>
<td>A</td>
<td>22.927</td>
<td>97.87</td>
<td>28954</td>
</tr>
<tr>
<td>B</td>
<td>2871.66</td>
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<tr>
<td>C</td>
<td>5</td>
<td>116.896</td>
<td>53654</td>
</tr>
<tr>
<td>ΔHV/(kJ mol(^{-1}))</td>
<td>132.128</td>
<td>83717</td>
<td>132.128</td>
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<tr>
<td>298 K</td>
<td>42.51</td>
<td>137.713</td>
<td>97604</td>
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<td>Linder 1931</td>
<td>Stuckey &amp; Saylor 1940</td>
<td></td>
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<tr>
<td>t/°C</td>
<td>P/Pa</td>
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<td>P/Pa</td>
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<td>eq. 4</td>
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<td>34897</td>
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<td>2871.66</td>
<td>110.041</td>
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<td>C</td>
<td>5</td>
<td>116.896</td>
<td>53654</td>
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<td>bp/°C</td>
<td>138.99</td>
<td>139.15</td>
<td>139.99</td>
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2.

<table>
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<td>summary of literature data</td>
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<td>selected values</td>
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<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
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**TABLE 3.1.1.5.2 (Continued)**

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**mp/°C** –47.9

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<th>t/°C</th>
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**bp/°C** 139.104

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**∆HV/(kJ mol⁻¹) =**

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**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 m-xylene at various temperatures and temperature dependence equations

\[
\ln K_{AW} = A - B/(T/K) \\
\ln (1/K_{AW}) = A - B/(T/K) \\
\ln (k_H/\text{atm}) = A - B/(T/K) \\
\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \\
K_{AW} = A - B(T/K) + C(T/K)^2
\]

Sanemasa et al. 1982  
Ashworth et al. 1988  
Robbins et al. 1993  
Dewulf et al. 1995

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Gruber et al. 1997

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<td>50.28</td>
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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

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<tr>
<td>20.29</td>
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<td>50.28</td>
<td>3.30</td>
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</table>
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: C₈H₁₀, C₆H₄(CH₃)₂  
Molecular Weight: 106.165  
Melting Point (°C):  
13.25  (Lide 2003)  
Boiling Point (°C):  
138.37  (Lide 2003)  
Density (g/cm³ at 20°C):  
0.8611  (Weast 1982–83)  
Molar Volume (cm³/mol):  
123.3  (20°C, calculated-density)  
140.4  (calculated-Le Bas method at normal boiling point)  
Enthalpy of Vaporization, ∆HV (kJ/mol):  
42.376, 35.98  (25°C, bp, Riddick et al. 1986)  
Enthalpy of Fusion ∆Hfus (kJ/mol):  
17.113  (Tsonopoulos & Prausnitz 1971; Riddick et al. 1986)  
17.11  (Chickos et al. 1999)  
Entropy of Fusion ∆Sfus (J/mol 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°C, F: 1.0  
Water Solubility (g/m³ or mg/L at 25°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°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°C, shake flask-UV, Ben-Naim & Wiff 1979)  
163*  (vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1982)  
214.5  (generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)  
182  (HPLC-κ′ correlation, converted from reported γₒ, 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°C, Shaw 1989b)  
169*  (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994c)  
ln x = 11.79 – 20.89·(T/K)⁻¹ + 4.892·(T/K)⁻²; Tᵣ = T/Tᵣ, the reduced temp, system temp T divided by critical temp Tᵣ, temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994c)  
ln x = −27.937 + 3230.3/(T/K) + 7.595 × 10⁻⁵·(T/K)²; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
Vapor Pressure (Pa at 25°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* (0.2°C, mercury manometer, Linder 1931)
787* (20°C, Hg manometer, Kassel 1936)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = -2930.0/(T/K) + 23.1000; \text{ temp range 0–80°C (vapor pressure eq. from Hg manometer measurements, Kassel 1936)} \]

1437* (30°C, Hg manometer, measured range 10–50°C, Rintelen et al. 1937)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = -2851.90/(T/K) + 22.88436; \text{ temp range 4–75°C (vapor pressure eq. from manometer measurement, Stuckey & Saylor 1940)} \]

1187* (Hg manometer, Pitzer & Scott 1943)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = -3141.33/(T/K) + 11.6092; \text{ temp range 0–13.23°C (manometer, solid, two-constant vapor pressure eq. from exptl. data, Pitzer & Scott 1943)} \]

\[ \log \left( \frac{P}{\text{mmHg}} \right) = -3080.31/(T/K) - 5 \log (T/K) + 27.8581; \text{ temp range 13.23–60°C (manometer, liquid, three-constant eq. from exptl. data, Pitzer & Scott 1943)} \]

6354* (58.288°C, ebulliometry, measured range 58.288–139.289°C, Willingham et al. 1945)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 6.98648 - 1491.548/(207.171 + t/°C); \text{ temp range 58.3–139.8°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)} \]

1333* (27.3°C, summary of literature data, Stull 1947)

6398* (58.419°C, ebulliometry, measured range 58.419–139.329°C, Forziati et al. 1949)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 6.99184 - 1454.328/(215.411 + t/°C); \text{ temp range 58.4–139.3°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)} \]

1175 (extrapolated-Antoine eq., Dreisbach 1955)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 6.99052 - 1453.430/(215.307 + t/°C); \text{ temp range 45–190°C (Antoine eq. for liquid state, Dreisbach 1955)} \]

126500* (146.85°C, ebulliometry, measured range 146.85–316.85°C, Ambrose et al. 1967)

1170* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 6.9052 - 1453.430/(215.307 + t/°C); \text{ temp range 27.32–166.73°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]

\[ \log \left( \frac{P}{\text{mmHg}} \right) = \left[-0.2185 \times 9809.9/(T/K)\right] + 8.124805; \text{ temp range –8.1 to 138.3°C (Antoine eq., Weast 1972–73)} \]


\[ \log \left( \frac{P}{\text{mmHg}} \right) = (1 – 411.503/T) \times 10^{(0.847730 – 6.39489 \times 10^{-4} \cdot T + 5.59094 \times 10^{-7} \cdot T^2)}; \text{ T in K, temp range 290.0–618.2 K (Cox vapor pressure eq., Chao et al. 1983)} \]

1170 (extrapolated-Antoine eq., Boublík et al. 1984)

\[ \log \left( \frac{P}{\text{kPa}} \right) = 6.11140 - 1451.39/(215.148 + t/°C); \text{ temp range not specified (Antoine eq., Riddick et al. 1986)} \]

1180 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log \left( \frac{P}{\text{atm}} \right) = (1 - 411.503/T) \times 10^{(0.847730 – 6.39489 \times 10^{-4} \cdot T + 5.59094 \times 10^{-7} \cdot T^2)}; \text{ T in K, temp range 247–286 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)} \]

\[ \log \left( \frac{P}{\text{atm}} \right) = 6.14779 - 1475.767/(–55.241 + t/°C); \text{ temp range 27–166°C (Antoine eq.-II, Stephenson & Malanowski 1987)} \]

\[ \log \left( \frac{P}{\text{atm}} \right) = 6.14049 - 1472.773/(–55.342 + t/°C); \text{ temp range 41–463 K (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)} \]

\[ \log \left( \frac{P}{\text{atm}} \right) = 6.44333 – 1375.196/(–19.846 + T/K); \text{ temp range 460–553 K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)} \]

\[ \log \left( \frac{P}{\text{atm}} \right) = 7.84182 – 3543.356/(208.522 + T/K); \text{ temp range 551–616 K (liquid, Antoine eq.-V, Stephenson & Malanowski 1987)} \]

1165* (McLeod gauge, measured range 20.0–50.07, Smith 1990)

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 60.0531 – 4.1059 \times 10^{3}/(T/K) – 19.441 \log (T/K) + 8.2881 \times 10^{3}\cdot(T/K) – 2.3647 \times 10^{-12}\cdot(T/K)^2; \text{ temp range 286–616 K (vapor pressure eq., Yaws 1994)} \]
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

762* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)
754*; 752 (EPICS-GC/FID; batch air stripping-GC, Ashworth et al. 1988)

\[ \ln \left( \frac{H}{(\text{atm} \cdot \text{m}^3/\text{mol})} \right) = 6.931 - \frac{3520}{(T/\text{K})}; \text{temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)} \]

614 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

856, 1189, 1576 (27 35.8 46°C, EPICS-GC, Hansen et al. 1993)

\[ \ln K_{AW} = -\frac{4479}{(T/\text{K})} + 0.01196\cdot Z + 13.597; \text{with } Z \text{ salinity 0–35.5‰, temp range 2–25°C (EPICS-GC/FID, Dewulf et al. 1995)} \]

696 (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°C, Dewulf et al. 1995)


Octanol/Water Partition Coefficient, log \( K_{OW} \) at 25°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 \( K_{OA} \) at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.68* (30.3°C, from GC-determined \( \gamma^* \) in octanol, measured range 30.3–50.28°C, Gruber et al. 1997)
3.79 (calculated-measured \( \gamma^* \) in pure octanol of Gruber et al. 1997, Abraham et al. 2001)

Bioconcentration Factor, log 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 \( K_{OC} \) at 25°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 \( f_{OC} \) of 0.006 and measured partition coeff. \( K_p = 1.04 \text{ mL/g.}, Abdul et al. 1990 \)
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-\( k' \) correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Vaprolization: $t_{1/2} \approx 3.1$ h for evaporation from water of 1 m depth with wind speed of 3 m/s and water current of 1 m/s/h (Lyman et al. 1982);

$\Delta t_{1/2} \approx 27–135$ h for evaporation from a typical river or pond (Howard 1990).

Photolysis:

Oxidation: rate constant $k$ for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO3 radical and $k_O$ with O3 or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

photooxidation $t_{1/2} = 2.8 \times 10^6–1.4 \times 10^8$ h, based on estimated rate data for alkoxy radical in aqueous solution (Hendry 1974)

$k_{OH} = (7.4 \pm 1.5) \times 10^6$ L mol$^{-1}$ s$^{-1}$;  $k_{O3/SP} = (1.09 \pm 0.11) \times 10^8$ L mol$^{-1}$ s$^{-1}$ with O(P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (12.2 \pm 1.2) \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$;  $k_{O3/SP} = (1.81 \pm 0.18) \times 10^{13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction of O(P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 7.45 \times 10^6$ L mol$^{-1}$ s$^{-1}$ with $t_{1/2} = 0.24–2.4$ h (Darnall et al. 1976)

$k_{OH} = (15.3 \pm 1.7) \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH} = (8.8–10.5) \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishanakara et al. 1978)

$k_{OH} = 12.3 \times 10^{12}$ cm$^3$ molecule$^{-1}$ 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)

$k_{OH} = 950$ cm$^3$ mol$^{-1}$ s$^{-1}$ at 300 K (Lyman et al. 1982)

$k_{OH} = (5.9–12) \times 10^9$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 0.47–1.0$ d for xylenes (Mill 1982)

$k = (140 \pm 30)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water using 1 mM $t$-BuOH as scavenger at pH 2.0 and 20–23°C (Hoigné & Bader 1983)

$k_{NO3} = 1.4 \times 10^{16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{OH} = 14.1 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with half-life of 4.2–42 h (Atkinson 1985; Howard et al. 1991)

$k_{OH} = 12.9 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C (Ohta & Ohyama 1985)

$k_{OH} = 13.6 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 22.8°C, with a calculated atmospheric lifetime $\tau = 0.84$ d (Edney et al. 1986)

$k_{OH}(calc) = 6.9 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(obs.) = 15.2 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{NO3} = 4.50 \times 10^{10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH} = 1.52 \times 10^{11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{OH} = 1.43 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ over temp range at 296–335 K (recommended, Atkinson 1989)

$k_{OH} = 14.3 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1990)

$k_{OH}(calc) = 6.92 \times 10^{11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH}(calc) = 17.40 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{OH}(calc) = 6.51 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(exptl) = 14.3 \times 10^{12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982)

$t_{1/2} = 1150$ months, abiotic hydrolysis or dehydro-halogenation half-life (Olsen & Davis 1990).

Biodegradation:

100% biodegraded after 192 h at 13°C with an initial concn of 1.03 × 10$^{-6}$ L/L (Jamison et al. 1976)

$t_{1/2}(aq. aqueous) = 168–672$ 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)

$t_{1/2}(aq. anaerobic) = 672–2688$ h, based on unacclimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991)

$t_{1/2} = 0.03$ d (Olsen & Davis 1990).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:
Half-Lives in the Environment:
Air: $t_{1/2} = 0.24–2.4$ 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 $t_{1/2} = 3.1$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976) $t_{1/2} = 4.2–42$ h, based on photooxidation half-life (Howard et al. 1991);
calculated atmospheric lifetime $\tau = 0.84$ d due to reaction with OH radical (Edney et al. 1986);
summer daylight lifetime $\tau = 10$ h due to reaction with OH radical (Altshuller 1991).
Surface Water: $t_{1/2} = 168–672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Ground water: $t_{1/2} = 336–8640$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991);
$\sim 0.3$ yr from observed persistence in groundwater of the Netherlands (Zoeteman et al. 1981);
abiotic hydrolysis or dehydro-halogenation $t_{1/2} = 1150$ months (Olsen & Davis 1990).
Soil: $t_{1/2} = 168–672$ h, based on estimated aqueous aerobic biodegradation half-life (Bridie et al. 1979; Kuhn et al. 1985; Howard et al. 1991);
disappearance $t_{1/2} = 2.2$ d from test soils (Anderson et al. 1991).
Biota: $t_{1/2} = 2.6$ d, half-life to eliminate from eels in seawater (Ogata & Miyake 1978).

### TABLE 3.1.1.6.1
Reported aqueous solubilities of $p$-xylene at various temperatures

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<td>$S/\text{g} \cdot \text{m}^{-3}$</td>
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$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.48$ at $25\degree\text{C}$

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.90$ at $25\degree\text{C}$

$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.20$ at $25\degree\text{C}$
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 p-xylene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) + D(T/K)^2 \quad (5)
\end{align*}
\]

1.

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<td>ΔH_f/(kJ mol⁻¹) = 42.30 at 298 K</td>
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(Continued)
### TABLE 3.1.1.6.2 (Continued)

3. Osborn & Douslin 1974

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Smith 1990

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McLeod gauge

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<td>44.27</td>
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∆HV/(kJ mol⁻¹) = 42.98

at 25°C

∆SV/(J mol⁻¹ K⁻¹) = 107.0

at 25°C

---

**FIGURE 3.1.1.6.2** Logarithm of vapor pressure versus reciprocal temperature for p-xylene.

---

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TABLE 3.1.1.6.3
Reported Henry’s law constants of \( p \)-xylene at various temperatures and temperature dependence equations

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<th>Temperature/Source</th>
<th>Henry’s Law Constant</th>
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<td>t/°C</td>
<td>H/Pa m³/mol</td>
<td>t/°C</td>
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**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

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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: \( \text{C}_9\text{H}_{12}, \text{C}_6\text{H}_3(\text{CH}_3)_3 \)
Molecular Weight: 120.191

Melting Point (°C):
-25.4  (Weast 1982–83; Lide 2003)

Boiling Point (°C):
176.1  (Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
0.8944  (Weast 1982–83)

Molar Volume (cm³/mol):
134.4  (20°C, calculated-density)
162.6  (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion \( \Delta H_{\text{fus}} \) (kJ/mol):
0.66, 1.33, 8.18, 10.17  (–54.45, –42.85, –25.35°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion \( \Delta S_{\text{fus}} \) (J/mol K):
41.81, 46.2  (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Sanemasa et al. 1982)
65.5  (generator column-HPLC/UV, Tewari et al. 1982c)
69*  (IUPAC recommended value, temp range 15–45°C, Shaw 1989b)

\[ \ln x = -39.5173 + 5289.13/(T/K) + 1.149 \times 10^{-4} \cdot (T/K)^2; \text{ temp range } 5-50°C \] (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°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*  (16.8°C, summary of literature data, Stull 1947)
6417*  (90.332°C, ebulliometry, measured range 90.332–177.126°C, Forziati et al. 1949)
log (P/mmHg) = 7.04082 – 1593.958/(207.078°C + t°C); temp range 90.3–177.1°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
206  (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.04082 – 1593.958/(207.078°C + t°C); temp range 75–230°C (Antoine eq. for liquid state, Dreisbach 1955)
198*  (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.04082 – 1593.958/(207.078°C + t°C); temp range 56.79–205.36°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [-0.2185 × 10^781.9/(T/K)] + 8.154069; temp range 16.8–176°C (Antoine eq., Weast 1972–73)
217  (calculated-bp, Mackay et al. 1982; Eastcott et al. 1988)
log (P/atm) = (1 – 449.175/T) × 10^6(0.869047 – 6.33423 × 10^4·T + 5.14963 × 10^7·T²); 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)
Mononuclear Aromatic Hydrocarbons

\[
\log (P_{/kPa}) = 6.16365 - 1592.422/(206.905 + t/°C); \text{ temp range 90.33–177.1°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublík et al. 1984)}
\]

198.4 \hspace{1cm} \text{(extrapolated-Antoine eq., Dean 1985, 1992)}

\[
\log (P_{/mmHg}) = 7.04082 - 1593.958/(207.08 + t/°C); \text{ temp range 57–205°C (Antoine eq., Dean 1985, 1992)}
\]

199 \hspace{1cm} \text{(extrapolated, Antoine eq., Stephenson & Malanowski 1987)}

\[
\log (P_{/kPa}) = 6.16477 - 1593.776/(-66.032 + T/K); \text{ temp range 363–456 K (Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log (P_{/mmHg}) = 2.7492 - 2.6428 \times 10^3/(T/K) + 3.6120 \times \log (T/K) - 1.0213 \times 10^{-2} \times (T/K) + 5.0553 \times 10^{-6} \times (T/K)^2, \text{ temp range 248–665 K (vapor pressure eq., Yaws 1994)}
\]

\[
\log (P_{/kPa}) = 6.17303 - 1593.958/[(T/K) - 66.072]; \text{ temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

441* \hspace{1cm} \text{(vapor-liquid equilibrium-GC, measured range 15–45°C, Sanemasa et al. 1982)}

364 \hspace{1cm} \text{(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)}

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

3.66 \hspace{1cm} \text{(Hansch & Leo 1979)}

3.66 \hspace{1cm} \text{(HPLC-k’ correlation, Hammers et al. 1982)}

3.55 \hspace{1cm} \text{(generator column-HPLC/UV, Tewari et al. 1982b, 1982c)}

3.70, 3.86 \hspace{1cm} \text{(RP-HPLC-k’ correlation, Sherblom & Eganhouse 1988)}

3.63 \hspace{1cm} \text{(recommended, Sangster 1989, 1993)}

3.55, 3.59, 3.66 \hspace{1cm} \text{(quoted lit. values, Hansch et al. 1995)}

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{OC} \):

2.80 \hspace{1cm} \text{(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, \( t_\text{½} \):

Vaporization:

Oxidation: rate constant \( k \); for gas-phase second-order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO₃ radical and \( k_{O3} \) with O₃ or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

\[
k_{OH} = (14 \pm 3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}; \quad k_{O(3P)} = (6.9 \pm 0.7) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with O(3P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)}
\]

\[
k_{OH} = (26.4 \pm 2.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \quad k_{O(3P)} = 11.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ for the reaction of O(3P) atom at room temp (flash photolysis-resonance fluorescence, Hansen et al. 1975)}
\]

\[
k_{OH} = 14.9 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with } t_\text{½} = 0.24–2.4 \text{ h (Darnall et al. 1976)}
\]

\[
k_{OH,*} = (33.3 \pm 4.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence Perry et al. 1977)}
\]

\[
k_{OH} = (15–30) \times 10^9 \text{ M}^{-1} \text{ s}^{-1} \text{ with } t_\text{½} = 0.2–0.4 \text{ d for trimethylbenzenes (Mill 1982)}
\]

\[
k = (400 \pm 100) \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone in water at pH 1.7 and 20–23°C (Hoigné & Bader 1983)}
\]

\[
k_{NO3} = 5.6 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 296 K (Atkinson et al. 1984)}
\]

\[
k_{OH} = 3.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1985)}
\]

\[
k_{OH} = 2.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (Ohta & Ohyama 1985)}
\]

\[
k_{OH} \text{(calc)} = 1.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \quad k_{OH} \text{(obs.)} = 3.33 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (SAR [structure-activity relationship], Atkinson 1987)}
\]

\[
k_{NO3} = 1.85 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}; \quad k_{OH} = 3.16 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)}
\]

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k_{OH} = 3.27 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989, 1990)}

k_{OH(\text{calc})} = 1.78 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (estimated by SARs, Müller & Klein 1992)}

k_{OH(\text{calc})} = 3.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}

Hydrolysis:

Biotransformation:

Biodegradation:

Bioconcentration:

Half-Lives in the Environment:

Air: \tau_a = 0.24–2.4 \text{ 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 \text{ h under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Perry et al. 1977); summer daylight lifetime } \tau = 4.2 \text{ h due to reaction with OH radical (Altshuller 1991)}

TABLE 3.1.1.7.1

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<th>t/°C</th>
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FIGURE 3.1.1.7.1 Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for 1,2,3-trimethylbenzene.
Reported vapor pressures of 1,2,3-trimethylbenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + T/K} \quad (2) \\
\ln P &= A - \frac{B}{C + T/K} \quad (2a) \\
\log P &= A - \frac{B}{C + \frac{T}{K}} \quad (3) \\
\ln P &= A - \frac{B}{C + \frac{T}{K}} - C \log \left(\frac{T}{K}\right) \quad (4)
\end{align*}
\]

Stull 1947
Forziati et al. 1949
Zwolinski & Wilhoit 1971

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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: C₉H₁₂, C₆H₃(CH₃)₃
Molecular Weight: 120.191
Melting Point (°C):
  –43.77 (Lide 2003)
Boiling Point (°C):
  169.38 (Lide 2003)
Density (g/cm³ at 20°C):
  0.8758 (Weast 1982–83)
Molar Volume (cm³/mol):
  137.2 (20°C, calculated-density)
  162.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH⁰ (kJ/mol):
  13.19 (Chickos et al. 1999)
Entropy of Fusion ΔS⁰ (J/mol K):
  57.53, 46.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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)
\[ \ln x = -8.760 - 868.70/(T/K); \text{ temp range } 5–50°C \] (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°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*  (13.6°C, summary of literature data, Stull 1947)
  6417*  (84.804°C, ebulliometry, measured range 84.804–170.377°C, Forziati et al. 1949)
\[ \log (P/mmHg) = 7.04393 - 1573.267/(208.564 + T/°C); \text{ temp range } 84.8–170.4°C \] (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
  280  (extrapolated-Antoine eq., Dreisbach 1955)
\[ \log (P/mmHg) = 7.04383 - 1573.267(208.564 + T/°C); \text{ temp range } 70–220°C \] (Antoine eq. for liquid state, Dreisbach 1955)
  2666*  (65.405°C, compiled data, temp range 65.405–198.215°C, Bond & Thodos 1960)
\[ \log (P/mmHg) = 23.2393 - 3301.19/(T/K) - 6.21412 \log (T/K) + 3.15835[P/mmHg]/(T/K)^2; \text{ temp range } 65.4–198°C \] (Bond & Thodos 1960)
\[ \log (P/mmHg) = 7.04383 - 1573.267(208.564 + T/°C); \text{ temp range } 51.75–198.2°C \] (Antoine eq., Zwolinski & Wilhoit 1971)

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log (P/mmHg) = [-0.2185 × 10710.2/(T/K)] + 8.209013; temp range 13.6–169.2°C (Antoine eq., Weast 1972–73)

log (P/atm) = (1 – 442.537/T) × 10^(0.846724 – 5.41424 × 10 4·T + 4.22211 × 10 7·T^2); T in K, temp range 253.0–645.0 K (Cox vapor pressure eq., Chao et al. 1983)

log (P/mmHg) = 7.04383 – 1573.83/(208.56 + t/°C); temp range 52–198°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 2.1667 – 2.6318 × 10 3/(T/K) + 4.0350·log (T/K) – 1.1776 × 10–2·(T/K) + 6.0956 × 10–6·(T/K)^2, temp range 229–649 K (vapor pressure eq., Yaws 1994)

log (P/kPa) = 6.16282 – 1569.06/(208.089 + t°c); temp range 84.8–170.4°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

log (P/kPa) = 6.16695 – 1572.687/(-64.593 + T/K); temp range 357–450 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 6.16866 – 1573.267/([T/K] – 64.586); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°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°C, Sanemasa et al. 1982)
475 (20°C, EPICS-GC, Yurteri et al. 1987)
571 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
704, 1135, 1591 (27, 35, 45°C, EPICS-GC, Hansen et al. 1993)

ln [H/(kPa·m³/mol)] = –4298/(T/K) + 14.0; temp range 27–45°C (EPICS-GC, Hansen et al. 1993)

529 (20°C, selected from literature experimentally measured data, Staudinger & Roberts, 1996, 2001)

log K_{AW} = 5.125 – 1697/(T/K) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{ow}:
3.65 (calculated-π 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-k’ correlation, Gover & Evers 1992)
3.70 (recommended, Sangster 1993)
3.83, 3.78 (quoted lit., Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:
3.28 (computed-K_{ow}, Kollig 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:
3.28 (computed-K_{ow}, Kollig 1995)

Environmental Fate Rate Constants, k, or Half-Lives, t_{½}:

Photolysis: rate constant k = 2.686 × 10^2 h^−1 with H₂O₂ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO3} with NO₃ radical and k_{O₃} with O₃, or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

k_{OH} = (2.0 ± 0.3) × 10^{10} L mol⁻¹ s⁻¹ with t_{½} = 0.58 h; k_{OH(3P)} = (6.0 ± 0.6) × 10^8 L mol⁻¹ s⁻¹ with O(³P) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

k_{OH} = (33.5 ± 3.4) × 10^{12} cm³ molecule⁻¹ s⁻¹, and k_{NO3} = 1.0 × 10^{13} cm³ molecule⁻¹ s⁻¹ for the reaction of O(³P) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

k_{OH} = 20 × 10^8 L mol⁻¹ s⁻¹ with t_{½} = 0.24–2.4 h (Darnall et al. 1976)

k_{OH}* = (40.0 ± 4.5) × 10^{12} cm³·molecule⁻¹·s⁻¹ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence Perry et al. 1977)
photooxidation $t_{1/2} = 1056–43000$ h in water, based on measured rate data with hydroxy radical in aqueous solution (Güesten et al. 1981).

$k_{OH} = 33.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ 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).

$k_{OH} = (1.5–30) \times 10^9$ M$^{-1}$ s$^{-1}$ with $t_u = 0.2–0.4$ d for trimethylbenzenes (Mill 1982).

$k_{NO_3} = 5.4 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson et al. 1984).

$k_{OH} = 38.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with $t_u = 1.6–16$ h (Atkinson 1985).

$k_{OH} = 31.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 25°C (Ohta & Ohyama 1985).

$k_{OH} = 18 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(obs.)} = 40 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987).

$k_{NO_3} = 1.80 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{OH} = 3.84 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992).

$k_{OH} = 32.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1990).

$k_{OH}^{(calc)} = 1.78 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992).

$k_{OH}^{(calc)} = 39.72 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993).

Hydrolysis: no hydrolyzable functional groups (Mabey et al. 1982).

Biodegradation: aqueous aerobic biodegradation $t_{1/2} = 168–672$ 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 $t_{1/2} = 672–2688$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Half-Lives in the Environment:

Air: $t_u = 0.58$ h estimated from the rate of disappearance for the reaction with OH radical (Doyle et al. 1975).

$t_u = 0.24–2.4$ 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).

$t_u = 1.6–16$ h, based on photooxidation half-life in air (Atkinson 1985; Howard et al. 1991); summer daylight lifetime $\tau = 4.3$ h due to reaction with OH radical (Altshuller 1991); calculated lifetimes of 4.3 h, 26 d and $> 4.5$ yr for reactions with OH radical, NO$_3$ radical and O$_3$, respectively (Atkinson 2000).


Photooxidation $t_u = 1056–43000$ h, based on measured rate data with OH radical in aqueous solution (Güesten et al. 1981; Howard et al. 1991).

Ground water: $t_u = 336–1344$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Soil: $t_u = 168–672$ 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 1,2,4-trimethylbenzene at various temperatures

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<th>Aqueous solubility</th>
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\[
\ln \left[ \frac{H}{(\text{kPa m}^3/\text{mol})} \right] = A - \frac{B}{T/\text{K}} \\
A = 14.0 \\
B = 4298
\]

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

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<td>(5) ( \log P = A - B/(T/\text{K}) - C \cdot \log (T/\text{K}) + D \cdot P/(T/\text{K})^2 )</td>
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<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
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**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: C₉H₁₂, C₆H₃(CH₃)₃
Molecular Weight: 120.191
Melting Point (°C):
-44.7 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
164.74 (Lide 2003)
Density (g/cm³ at 20°C):
0.880 (Weast 1982–83)
Molar Volume (cm³/mol):
136.6 (20°C, calculated-density)
162.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ∆HV (kJ/mol):
47.48, 39.04 (25°C, bp, Riddick et al. 1986)
51.85 (calculated-bp, Govers & Evers 1992)
Enthalpy of Fusion ∆Hfus (kJ/mol):
9.514 (Riddick et al. 1986)
9.51 (Chickos et al. 1999)
Entropy of Fusion ∆Sfus (J/mol K):
41.66, 46.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Sanemasa et al. 1981)
50* (vapor saturation-UV, temp range 15–45°C, Sanemasa et al. 1982)
49.5 (HPLC-k' correlation, converted from reported γW, Hafkenscheid & Tomlinson 1983)
48.9* (recommended, temp range 15–45°C, Shaw 1989b)
64* (30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994c)
ln x = 26.26 – 35.26·(T/K)⁻¹ + 7.905·(T/K)⁻²; T = T/Tc, the reduced temp, system temp T divided by critical temp Tc, temp range 303.15–373.15 K (equilibrium flow cell-GC, Chen & Wagner 1994c)
ln x = -9.533 – 678.83/(T/K); temp range 0–80°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°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* (10.6°C, mercury manometer, Linder 1931)
248* (20°C, mercury manometer, Kassel 1936)
log (P/mmHg) = -3104.5/(T/K) – 5·log (T/K) + 23.1929; temp range 0–80°C (vapor pressure eq. from Hg manometer measurements, Kassel 1936)
507* (30°C, mercury manometer, measured range 10–50°C, Rintelen et al. 1937)
Mononuclear Aromatic Hydrocarbons

log (P/mmHg) = –3122.45/(T/K) – 5·log (T/K) + 22.2368; temp range 4–75°C (manometer, vapor pressure eq. from exptl. data, Stuckey & Saylor 1940)

133.3* (9.6°C, summary of literature data, Stull 1947)

6415* (81.488°C, ebulliometry, measured range 81.488–165.725°C, Forziati et al. 1949)

log (P/mmHg) = 7.07437 – 1569.622/(209.578 + t/°C); temp range 81.5–165.7°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

331 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 7.07436 – 1569.622/(209.58 + t/°C); temp range 49–193°C (Antoine eq., Dean 1985, 1992)

330 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/mmHg) = 7.07436 – 1569.622/(209.578 + t/°C); temp range 70–210°C (Antoine eq. for liquid state, Dreisbach 1955)

328* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981; Eastcott et al. 1988)

log (P/mmHg) = 7.07435 – 1569.622/(209.578 + t/°C); temp range 48.82–193.07°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 10516.8/(T/K)] + 8.161663; temp range 9.6–164.7°C (Antoine eq., Weast 1972–73)

366 (calculated-bp, Mackay et al. 1982)

log (P/atm) = (1 – 437.769/T) × 10^(0.872945 – 6.55508 × 10^4·T + 5.47586 × 10^7·T^2); 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 (P/kPa) = 6.20212 – 1571.575/(209.79 + t/°C); temp range 81.488–165.7°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 (P/kPa) = 6.21017 – 1577.80/(210.526 + t/°C); temp range not specified (Antoine eq., Riddick et al. 1986)

log (P/mmHg) = 7.07436 – 1569.622/(209.58 + t/°C); temp range 49–193°C (Antoine eq., Dean 1985, 1992)

330 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

log (P/kPa) = 6.19762 – 1569.749/(–63.565 + T/K); temp range 354–445 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)

log (P/kPa) = 6.62312 – 1810.653/(–43.307 + T/K); temp range 249–356 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

360 (computed-expert system SPARC, Kollig 1995)

log (P/kPa) = 6.18965 – 1569.622/[T(K) ± 63.572]; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):


887* (vapor-liquid equilibrium, measured range 15–45°C, Sanemasa et al. 1982)

682; 849 (EPICS; batch stripping, Ashworth et al. 1988)

682* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm m³/mol)] = 7.241 – 3628/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

803 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

704 (infinite activity coeff. γ∞ in water determined by inert gas stripping-GC, Li et al. 1993)

597 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log K_AW = 4.329 – 1448/(T/K) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_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-k’ correlation, Govers & Evers 1992)

3.42 (recommended value, Sangster 1993)

3.42 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

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-$K_{OW}$, Kollig 1995)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Vaporization:

Photolysis: rate constant $k = 1.606 \times 10^{-2}$ h$^{-1}$ with $H_2O_2$ under photolysis at 25°C in F-113 solution and with $HO$ in the gas (Dilling et al. 1988).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O3} < 60$ L mol$^{-1}$ s$^{-1}$ for vapor phase reaction with ozone at 30°C (Bufalini & Altshuller 1965)

$k_{OH} = (31 \pm 4) \times 10^9$ L mol$^{-1}$ s$^{-1}$; $k_{OH(3P)} = (16.8 \pm 2.0) \times 10^9$ L mol$^{-1}$ s$^{-1}$ with O($^3P$) atom at room temp. (relative rate method, Doyle et al. 1975; Lloyd et al. 1976)

$k_{OH} = (47.2 \pm 4.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{D(3P)} = (27.9 \pm 3.3) \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the reaction of O($^3P$) atom at room temp. (flash photolysis-resonance fluorescence, Hansen et al. 1975)

$k_{OH} = 29.7 \times 10^9$ L mol$^{-1}$ s$^{-1}$ with $t_{1/2} = 0.24$–2.4 h (Darnall et al. 1976)

$k_{OH} = (62.4 \pm 7.5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp., measured range 296–473 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

photooxidation in water, $t_{1/2} = 3208$–1.28 $\times 10^5$ h, based on measured rate constant for reaction with hydroxyl radical in water (Mill et al. 1980)

$k_{OH} = 49.3 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ 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)

$k_{O3} = 4200$ cm$^3$ mol$^{-1}$ s$^{-1}$ for the reaction with ozone at 300 K (Lyman et al. 1982)

$k_{OH} = (15–30) \times 10^8$ M$^{-1}$ s$^{-1}$ with $t_{1/2} = 0.2$–0.4 d for trimethylbenzenes (Mill 1982)

$k = (700 \pm 200)$ M$^{-1}$ s$^{-1}$ for the reaction with ozone in water at pH 1.7 and 20–23°C (Hoigné & Bader 1983)

$k_{NO3} = 2.4 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson et al. 1984)

$k_{OH} = 60.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Atkinson 1985)

$k_{OH} = 38.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (Ohta & Ohyama 1985)

$k_{NO3} = 7.91 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and $k_{OH} = 6.05 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1985; Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1992)

$k_{OH(calc)} = 38 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH(obs.)} = 62.4 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{OH} = 57.5 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH(calc)} = 3.72 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (estimated by SARs, Müller & Klein 1992)

$k_{OH(calc)} = 54.16 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation: unacclimated aerobic aqueous biodegradation $t_{1/2} = 48$–192 h, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991); $t_{1/2}$(aq. anaerobic) = 192–768 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biocaccumulation:

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).

$t_{1/2} = 9.72-97.2$ h, based on estimated photooxidation half-life in air (Atkinson 1987).

Surface Water: $t_{1/2} = 48-192$ h, based on a soil column study in which aerobic groundwater was continuously percolated through quartz sand (Kappeler & Wuhrmann 1978; Howard et al. 1991);

Ground water: $t_{1/2} = 96-384$ 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: $t_{1/2} = 48-192$ 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

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$\Delta H_{sol}/(kJ \cdot mol^{-1}) = 4.49$ at 25°C

**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

\[
\text{log } P = A - B/(T/K) \quad (1) \\
\text{ln } P = A - B/(T/K) \quad (1a) \\
\text{log } P = A - B/(C + t/°C) \quad (2) \\
\text{ln } P = A - B/(C + t/°C) \quad (2a) \\
\text{log } P = A - B/(C + T/K) \quad (3) \\
\text{log } P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\]

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Mononuclear Aromatic Hydrocarbons

1,3,5-Trimethylbenzene: vapor pressure vs. 1/T

**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

\[
\begin{align*}
\ln K_{AW} &= A - B/(T/K) \\
\ln (1/K_{AW}) &= A - B/(T/K) \\
\ln (k_H/\text{atm}) &= A - B/(T/K) \\
\ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) \\
K_{AW} &= A - B(T/K) + C(T/K)^2
\end{align*}
\]

Sanemasa et al. 1981

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Sanemasa et al. 1982

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EPICS-GC

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A 7.241
B 3628

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FIGURE 3.1.19.3 Logarithm of Henry's law constant versus reciprocal temperature for 1,3,5-trimethylbenzene.
3.1.1.10  \textit{n-Propylbenzene}

\begin{figure}
\centering
\includegraphics[width=0.2\textwidth]{n-propylbenzene.png}
\caption{n-Propylbenzene}
\end{figure}

Common Name: \textit{n-Propylbenzene}

Synonym: 1-phenylpropane, propylbenzene

Chemical Name: \textit{n-propylbenzene}

CAS Registry No: 103-65-1

Molecular Formula: C$_9$H$_{12}$, C$_6$H$_5$(CH$_2$)$_2$CH$_3$

Molecular Weight: 120.191

Melting Point (°C):
-99.6  \textit{(Lide 2003)}

Boiling Point (°C):
159.24  \textit{(Lide 2003)}

Density (g/cm$^3$ at 20°C):
0.862  \textit{(Weast 1982–83)}

Molar Volume (cm$^3$/mol):
139.4  \textit{(20°C, calculated-density)}
170.0  \textit{(calculated-Le Bas method at normal boiling point)}

Enthalpy of Fusion $\Delta H_{\text{fus}}$ (kJ/mol):
9.27  \textit{(Chickos et al. 1999)}

Entropy of Fusion $\Delta S_{\text{fus}}$ (J/mol K):
53.39, 59.3  \textit{(exptl., calculated-group additivity method, Chickos et al. 1999)}

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

60  \textit{(15°C, volumetric, Fühner 1924; quoted, Chiou et al. 1982; Chiou 1985)}
120  \textit{(shake flask-turbidimetric, Stearns et al. 1947)}
55  \textit{(shake flask-UV, Andrews & Keffer 1950)}
120  \textit{(shake flask-UV, Klevens 1951)}
60  \textit{(shake flask-GC, Hermann 1972)}
70  \textit{(shake flask-GC, Krasnoshchekova & Gubergrits 1975)}
66.4  \textit{(shake flask-UV spec., Ben-Naim & Wiff 1979)}
51.9*  \textit{(generator column-HPLC/UV, 15–30°C, DeVoe et al. 1981)}
51.0*  \textit{(vapor saturation-UV spec., measured range 15–45°C, Sanemasa et al. 1982)}
47.1  \textit{(generator column-HPLC/UV, Tewari et al. 1982a)}
52.2  \textit{(generator column-HPLC/UV, GC/ECD, Tewari et al. 1982c)}
59.5  \textit{(HPLC-$k^\prime$ correlation, converted from reported $\gamma_W$, Hafkenscheid & Tomlinson 1983a)}
52.1  \textit{(generator column-HPLC/UV, Wasik et al. 1983)}
45.2  \textit{(vapor saturation-UV spec., Sanemasa et al. 1984)}
51.7*  \textit{(generator column-HPLC/UV, measured range 10–45°C, Owens et al. 1986)}
55.0*  \textit{(IUPAC recommended, temp range 15–45°C, Shaw 1989b)}
48.2*  \textit{(vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)}
55.0*  \textit{(shake flask-UV, measured range 0–50°C, Sawamura et al. 2001)}

\[ \ln x = -304.679 + 12774.71/(T/K) + 43.8994 \ln (T/K); \text{ temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)} \]

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):

260*  \textit{(13.9°C, mercury manometer, Linder 1931)}
6353*  \textit{(75.646°C, ebulliometry, measured range 75.646–160.202°C, Willingham et al. 1945)}
log (P/mmHg) = 6.95178 – 1649.548/(207.171 + t°C); temp range 75.6–160.2°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)

667* (31.3°C, summary of literature data, Stull 1947)

6402* (75.818°C, ebulliometry, measured range 75.818–160.239°C, Forziati et al. 1949)

log (P/mmHg) = 6.95094 – 1490.963/(207.100 + t/°C); temp range 75.8–160.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)

458 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 6.95142 – 1491.297/(207.140 + t/°C); temp range 75.2–160.2°C (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

log (P/kPa) = 6.08028 – 1493.914/(207.427 + t°C); temp range 75.2–160.24°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/mmHg) = 6.95142 – 1491.297/(207.14 + t/°C); temp range 43–188°C (Antoine eq., Dean 1985, 1992)

449* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 6.95142 – 1491.297/(207.14 + t/°C); temp range 43.33–187.87°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 10424.1/(T/K)] + 8.185880; temp range 6.3–159.2°C (Antoine eq., Weast 1972–73)

log (P/atm) = (1 – 432.321/T) × 10^(0.891023 – 6.89092 × 10 4·T + 5.79948 × 10 7·T^2); 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)

Henry’s Law Constant (Pa m³/mol at 25°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°C, Sanemasa et al. 1982)

1094* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

ln [H/(atm·m³/mol)] = 7.835 – 3681/(T/K), temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

1034 (calculated-vapor liquid equilibrium (VLE) data, Yaws et al. 1991)

1102 (infinite activity coeff. γ∞ in water determined by inert gas stripping-GC, Li et al. 1993)

1175* (equilibrium headspace-GC, measured range 10–30°C, Perlinger et al. 1993)

902 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

log K_AW = 4.587 – 1471/(T/K) (van’t Hoff eq. derived from lit. data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{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)


3.71 (generator column-HPLC/UV both phases, Tewari et al. 1982a)

3.63 (HPLC-k’ correlation, Hammers et al. 1982)

3.69 (generator column-HPLC/UV both phases, Tewari et al. 1982b, c; Wasik et al. 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-k’ 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, $\log K_{OA}$ at 25°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, $\log K_{OC}$:

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, $t_\text{½}$:

Volatilization: rate constants: $k = 0.037 \text{ d}^{-1}$, $t_\text{½} = 19 \text{ d}$ in spring at 8–16°C, $k = 0.539 \text{ d}^{-1}$, $t_\text{½} = 1.3 \text{ d}$ in summer at 20–22°C, $k = 0.065 \text{ d}^{-1}$, $t_\text{½} = 11 \text{ d}$ in winter at 3–7°C for the periods when volatilization appears to dominate, and $k = 0.086 \text{ d}^{-1}$, $t_\text{½} = 8.1 \text{ d}$ with HgCl$_2$ in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983)

Photolysis: rate constant $k = 6.96 \times 10^{-3} \text{ h}^{-1}$ with H$_2$O$_2$ under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO3}}$ with NO$_3$ radical and $k_{\text{O3}}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 3.7 \times 10^{9} \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_\text{½} = 2.4–24 \text{ h}$ (Darnall et al. 1976)

$k_{\text{OH}} = (3.7 \pm 0.8) \times 10^{9} \text{ L mol}^{-1} \text{ s}^{-1}$ at 305 ± 2 K (relative rate method, Lloyd et al. 1976)

$k_{\text{OH}} = (6.40, 5.86) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with different dilute gas, Ar or He at 298 K (flash photolysis-resonance fluorescence, Ravishanakara et al. 1978)

$k_{\text{OH}} = 3.5 \times 10^{-9} \text{ M}^{-1} \text{ s}^{-1}$ with $t_\text{½} = 1.6 \text{ d}$ (Mill 1982)

$k_{\text{OH}} = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}} = 6.58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Ohta & Ohyama 1985)

$k_{\text{OH}}(\text{calc}) = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR [structure-activity relationship], Atkinson 1987)

$k_{\text{OH}} = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}}(\text{calc}) = 5.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

Air: $t_\text{½} = 2.4–24 \text{ h}$, based on rate of disappearance for the reaction with hydroxyl radical (Danrall et al. 1976; Howard et al. 1991); estimated lifetime $\tau = 6 \text{ h}$ under photochemical smog conditions in S.E. England (Brice & Derwent 1978; Darnall et al. 1976).

Surface water: $t_\text{½} = 19 \text{ d}$ in spring at 6–16°C, $t_\text{½} = 1.3 \text{ d}$ in summer at 20–22°C, $t_\text{½} = 11 \text{ d}$ in winter at 3–7°C when volatilization dominates and $t_\text{½} = 8.1 \text{ d}$ with HgCl$_2$ in marine mesocosm experiments (Wakeham et al. 1983)
TABLE 3.1.1.10.1
Reported aqueous solubilities of \( n \)-propylbenzene at various temperatures

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<th>t/°C</th>
<th>S/g·m(^{-3} )</th>
<th>t/°C</th>
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\( \Delta H_{sol}/(kJ \text{ mol}^{-1}) = 3.70 \)

25°C

2. 

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<tr>
<td>55</td>
<td>74.4</td>
<td>30</td>
<td>56.2</td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

\( \Delta H_{sol}/(kJ \text{ mol}^{-1}) = 6.20 \)

25°C

FIGURE 3.1.1.10.1 Logarithm of mole fraction solubility (ln \( x \)) versus reciprocal temperature for \( n \)-propylbenzene.
TABLE 3.1.10.2
Reported vapor pressures of \(n\)-propylbenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C\log(T/K)
\end{align*}
\]

\[\text{(1)} \quad \text{ln } P = A - B/(T/K) \quad \text{(1a)}\]
\[\text{(2)} \quad \text{ln } P = A - B/(C + t/°C) \quad \text{(2a)}\]
\[\text{(3)} \quad \text{ln } P = A - B/(C + T/K) \quad \text{(3a)}\]
\[\text{(4)} \quad \text{ln } P = A - B/(T/K) - C\log(T/K) \quad \text{(4a)}\]

<table>
<thead>
<tr>
<th>Linder 1931</th>
<th>Willingham et al. 1945</th>
<th>Stull 1947</th>
<th>Forziati et al. 1949</th>
<th>Zwolinski &amp; Wilhoit 71</th>
</tr>
</thead>
<tbody>
<tr>
<td>mercury manometer</td>
<td>ebulliometry</td>
<td>summary of lit. data</td>
<td>ebulliometry</td>
<td>selected values</td>
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<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>---</td>
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<td>157.76</td>
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<td>157.76</td>
</tr>
<tr>
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<td>158.389</td>
<td>99203</td>
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<td>160.202</td>
<td>103910</td>
<td>105.085</td>
<td>19946</td>
<td>105.085</td>
</tr>
</tbody>
</table>

\[\text{bp/°C} \quad 159.218 \quad \Delta H_v/(kJ \text{ mol}^{-1}) = \]
| bp/°C | 159.216 |
|---|---|---|---|---|

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**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

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log K&lt;sub&gt;OW&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sanemasa et al. 1982</td>
<td></td>
</tr>
<tr>
<td>Ashworth et al. 1988</td>
<td></td>
</tr>
<tr>
<td>Perlinger et al. 1993</td>
<td></td>
</tr>
<tr>
<td>DeVoe et al. 1981</td>
<td></td>
</tr>
<tr>
<td>vapor-liquid equilibrium</td>
<td>EPICS-GC</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m&lt;sup&gt;3&lt;/sup&gt;/mol)</td>
</tr>
<tr>
<td>15</td>
<td>594</td>
</tr>
<tr>
<td>25</td>
<td>1062</td>
</tr>
<tr>
<td>35</td>
<td>1818</td>
</tr>
<tr>
<td>45</td>
<td>2754</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\ln H = A - \frac{B}{T/K}
\]

\[
H/(\text{atm m}^3/\text{mol})
\]

\[
A = 7.835
\]

\[
B = 3681
\]

Experimental data
Shull 1947
Zwolinski and Wilhoit 1971

b.p. = 159.24 °C
FIGURE 3.1.10.3 Logarithm of Henry’s law constant and $K_{OA}$ 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: C₉H₁₂, C₆H₅CH(CH)₂
Molecular Weight: 120.191
Melting Point (°C):
-96.02 (Lide 2003)
Boiling Point (°C):
152.41 (Lide 2003)
Density (g/cm³ at 20°C):
0.8618 (Weast 1982–83)
Molar Volume (cm³/mol):
139.5 (20°C, calculated-density)
162.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
45.141, 37.53 (25°C, bp, Riddick et al. 1986)
Enthalpy of Fusion ΔHfus (kJ/mol):
7.786 (Riddick et al. 1986)
7.32 (Chickos et al. 1999)
Entropy of Fusion ΔSfus (J/mol K):
41.34, 46.3 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°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 & Szegi 1978)
61.5* (vapor saturation-UV, measured range 15–45°C, Sanemasa et al. 1982)
56* (IUPAC recommended, temp range 15–80°C, Shaw 1989b)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
300* (13.7°C, mercury manometer, measured range –8.2–13.7°C, Linder 1931)
log (P/mmHg) = −2175/(T/K) + 7.991 (isoteniscope method, temp range not specified, Kobe et al. 1941)
6353* (70.02°C, ebulliometry, measured range 70.02–153.367°C, Willingham et al. 1945)
log (P/mmHg) = 6.92929 – 1455.811/(207.202 + t/°C); temp range 70.2–153.4°C (manometer, Antoine eq. from exptl. data, Willingham et al. 1945)
666.6* (31.3°C, summary of literature data, temp range 6.3–159.2°C, Stull 1947)
6401* (70.16°C, ebulliometry, measured range 70.16–153.4°C, Forzati et al. 1949)
log (P/mmHg) = 6.93958 – 1462.717/(207.993 + t/°C); temp range 70.2–153.4°C (manometer, Antoine eq. from exptl. data, Forzati et al. 1949)
Mononuclear Aromatic Hydrocarbons

log \( P/(\text{mmHg}) = 6.93666 – 1460.793/(207.777 + t/^\circ\text{C}) \); temp range 60–200\(^\circ\text{C}\) (Antoine eq., Dreisbach 1955)

609 (interpolated, Glew & Robertson 1956)

611* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

log \( P/(\text{mmHg}) = 6.93666 – 1460.793/(207.777 + t/^\circ\text{C}) \); temp range 38.29–180.67\(^\circ\text{C}\) (Antoine eq., Zwolinski & Wilhoit 1971)

\[
\log (P/kPa) = \left[-0.2185 \times 10^{335.3/(T/K)}\right] + 8.231760; \text{ temp range 2.9–152.4\(^\circ\text{C}\)} \quad \text{(Antoine eq., Weast 1972–73)}
\]

\[
\log (P/\text{atm}) = (1 – 425.438/T) \times 10^{(0.877964 – 7.34971 \times 10^{-4}\cdot T + 6.06942 \times 10^{-7}\cdot T^2)}; \ T \text{ in K, temp range 264.95–630.0 K} \quad \text{(Cox vapor pressure eq., Chao et al. 1983)}
\]

610 (extrapolated-Antoine eq., Boublik et al. 1984)

log \( P/(\text{mmHg}) = 6.0571 – 1457.715/(207.415 + t/^\circ\text{C}) \); temp range 70.02–153.4\(^\circ\text{C}\) (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

\[
\log (P/kPa) = 6.06528 – 1464.366/(208.235 + t/^\circ\text{C}) \quad \text{temp range 56.39–151.69\(^\circ\text{C}\)} \quad \text{(Antoine eq. from reported exptl. data of Dreyer et al. 1955, Boublik et al. 1984)}
\]

610 (selected lit., Riddick et al. 1986)

log \( P/(\text{mmHg}) = 6.06588 – 1464.17/(208.207 + t/^\circ\text{C}) \); temp range not specified (Antoine eq., Dean 1985, 1992)

log \( P/(\text{mmHg}) = 6.06586 – 1460.793/(207.78 + t/^\circ\text{C}) \); temp range 39–181\(^\circ\text{C}\) (Antoine eq., Dean 1985, 1992)

log \( P/(\text{mmHg}) = 6.06588 – 1464.17/(208.207 + t/^\circ\text{C}) \); temp range not specified (Antoine eq., Dean 1985, 1992)

log \( P/(\text{mmHg}) = 6.06586 – 1460.793/(207.78 + t/^\circ\text{C}) \); temp range 39–181\(^\circ\text{C}\) (Antoine eq., Dean 1985, 1992)

log \( P/(\text{mmHg}) = 6.06528 – 1464.366/(208.235 + t/^\circ\text{C}) \); temp range 70.02–153.4\(^\circ\text{C}\) (Antoine eq. from reported exptl. data of Forziati et al. 1949, Boublik et al. 1984)

\[
\log (P/kPa) = 6.06528 – 1464.366/(208.235 + t/^\circ\text{C}) \quad \text{temp range 56.39–151.69\(^\circ\text{C}\)} \quad \text{(Antoine eq. from reported exptl. data of Dreyer et al. 1955, Boublik et al. 1984)}
\]

610 (selected lit., Riddick et al. 1986)

Henry’s Law Constant (Pa m³/mol at 25°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* (28°C, EPICS-GC, measured range 28–46.1°C, Hansen et al. 1993)

\[
\ln \left[H/(kPa\cdot m^3/mol)\right] = –3269/(T/K) + 11.0; \text{ temp range 28–46.1°C} \quad \text{(EPICS-GC, Hansen et al. 1993)}
\]

1126 (infinite activity coeff. \( \gamma^\infty \) in water determined by inert gas stripping-GC, Li et al. 1993)

960 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)

902 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)

log \( K_{AW} = 3.774 – 1256/(T/K) \) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

3.43 (calculated-\( \pi \) substituent constant, Hansch et al. 1968)

3.66 (Leo et al. 1971; Hansch & Leo 1979)

3.62 (shake flask-GC, Chiu et al. 1977, 1982)

3.51 (headscape 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, Shierblom & Eganhouse 1988)

3.66 (recommended, Sangster 1989, 1993)

3.82 (from measured activity coeff., Tse et al. 1994)

3.66 (recommended, Hansch et al. 1993)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°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 \( K_{OC} \):

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Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

**Volutilization**: \( t_{1/2} = 5.7 \) h from water depth of 1 m (calculated, Mackay & Leinonen 1975).

**Photolysis**:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with \( \text{NO}_3 \) radical and \( k_{\text{O}_3} \) with \( \text{O}_3 \) or as indicated, *data at other temperatures see reference:

\[
k_{\text{OH}} = (3.7 \pm 0.8) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at } 305 \pm 2 \text{ K} \text{ (relative rate method, Lloyd et al. 1976)}
\]

\[
k_{\text{OH}} = 3.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ with } t_{1/2} = 2.4-24 \text{ h} \text{ (Darnall et al. 1976)}
\]

\[
k_{\text{OH}} = (7.79 \pm 0.40) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 200 \text{ torr He and } 298 \text{ K} \text{ (flash photolysis-resonance fluorescence, Ravishankara et al. 1978)}
\]

\[
k_{\text{OH}} = 4.6 \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1} \text{ with } t_{1/2} = 1.2 \text{ d} \text{ (Mill 1982)}
\]

\[k = (11 \pm 3) \text{ M}^{-1} \text{ s}^{-1} \text{ for the reaction with ozone in water using 100 mM } t\text{-BuOH as scavenger at pH } 2.0 \text{ and } 20-23^\circ\text{C} \text{ (Hoigné & Bader 1983)}
\]

\[
k_{\text{OH}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \text{ (Atkinson 1985)}
\]

\[
k_{\text{OH}} = 6.25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \text{ (relative rate method, Ohta & Ohyama 1985)}
\]

\[
k_{\text{OH}}^{\text{(calc)}} = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{\text{OH}}^{\text{(obs.)}} = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp.} \text{ (SAR [structure-activity relationship], Atkinson 1987)}
\]

\[
k_{\text{OH}} = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K} \text{ (recommended, Atkinson 1989, 1990)}
\]

\[
k_{\text{OH}}^{\text{(calc)}} = 4.69 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}
\]

Hydrolysis:

Biodegradation:

Bioconcentration

Half-Lives in the Environment:

Air: \( t_{1/2} = 2.4-24 \) h, based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991):

estimated lifetime \( \tau = 6 \) h under photochemical smog conditions in S.E. England (Brice & Derwent 1978) and (Darnall et al. 1976).

Surface Water: \( t_{1/2} = 5.79 \) h, calculated half-life based on evaporative loss at 25°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

<table>
<thead>
<tr>
<th></th>
<th>Aqueous solubility</th>
<th>Henry’s law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>shake flask-UV spec.</td>
<td>vapor equilibrium-UV spec.</td>
</tr>
<tr>
<td>( t/°C )</td>
<td>( S/\text{g·m}^{-3} )</td>
<td>( \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) )</td>
</tr>
<tr>
<td>24.936</td>
<td>80.47</td>
<td>15</td>
</tr>
<tr>
<td>29.984</td>
<td>82.91</td>
<td>25</td>
</tr>
<tr>
<td>34.918</td>
<td>85.64</td>
<td>35</td>
</tr>
<tr>
<td>39.958</td>
<td>89.79</td>
<td>45</td>
</tr>
<tr>
<td>44.905</td>
<td>94.57</td>
<td>50</td>
</tr>
<tr>
<td>49.902</td>
<td>100.4</td>
<td>( \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 5.10 )</td>
</tr>
<tr>
<td>54.916</td>
<td>106.9</td>
<td>at 25°C</td>
</tr>
<tr>
<td>59.983</td>
<td>115</td>
<td></td>
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<tr>
<td>65.165</td>
<td>124.4</td>
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<tr>
<td>70.32</td>
<td>135.6</td>
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<tr>
<td>75.097</td>
<td>147.3</td>
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<tr>
<td>80.209</td>
<td>161.7</td>
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</tr>
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</table>

\( \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 3.57 \) at 25°C
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

<table>
<thead>
<tr>
<th></th>
<th>log $P = A - B/(T/K)$</th>
<th>ln $P = A - B/(T/K)$</th>
<th>log $P = A - B/(C + t/°C)$</th>
<th>ln $P = A - B/(C + t/°C)$</th>
<th>log $P = A - B/(C + T/K)$</th>
<th>log $P = A - B/(T/K) - C\cdot\log (T/K)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linder 1931</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$t/°C$</td>
<td>$P$/Pa</td>
<td>$t/°C$</td>
<td>$P$/Pa</td>
<td>$t/°C$</td>
<td>$P$/Pa</td>
<td>$t/°C$</td>
</tr>
<tr>
<td>-8.2</td>
<td>57.3</td>
<td>70.02</td>
<td>6353</td>
<td>70.16</td>
<td>6401</td>
<td>36.29</td>
</tr>
<tr>
<td>1.3</td>
<td>124</td>
<td>74.365</td>
<td>7654</td>
<td>74.47</td>
<td>7693</td>
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</tr>
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<td>13.7</td>
<td>300</td>
<td>78.155</td>
<td>8965</td>
<td>78.23</td>
<td>8993</td>
<td>59.79</td>
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<td>81.579</td>
<td>10304</td>
<td>84.768</td>
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<td>84.91</td>
<td>11722</td>
<td>66.06</td>
</tr>
<tr>
<td>89.077</td>
<td>16621</td>
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Stull 1947

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Forziati et al. 1949

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Zwolinski & Wilhoit 1971

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$\Delta H_v$/(kJ mol$^{-1}$) =

at 25°C 45.14
at bp 37.53

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FIGURE 3.1.11.2 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: C₉H₁₂, C₆H₄CH₃C₂H₅
Molecular Weight: 120.191
Melting Point (°C): –79.83 (Lide 2003)
Boiling Point (°C): 165.2 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C): 0.8807 (Weast 1982–83)
Molar Volume (cm³/mol): 136.5 (20°C, calculated-density)
                         162.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ∆Hₓ (kJ/mol): (Lide 2003)
Entropy of Fusion ∆Sₓ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
                              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°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* (9.4°C, summary of literature data, Stull 1947)
                              log (P/mmHg) = 7.00314 – 1535.374/(207.300 + t°C); temp range 81.1–166.2°C (manometer, Antoine eq. from
                              exptl. data, Forziati et al. 1949)
                              336 (extrapolated-Antoine eq., Dreisbach 1955)
                              log (P/mmHg) = 7.00314 – 1535.374/(207.3 + t°C); temp range 70–215°C (Antoine eq. for liquid state, Dreisbach 1955)
                              330* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
                              log (P/mmHg) = 7.00314 – 1535.374/(207.300 + t°C); temp range 48.46–193.89°C (Antoine eq., Zwolinski &
                              Wilhoit 1971)
                              log (P/mmHg) = [−0.2185 × 10448.8/(T/K)] + 8.141032; temp range 9.4–165.2°C (Antoine eq., Weast 1972–73)
                              log (P/atm) = (1 – 438.357/T) × 10¹⁵(0.863837 – 6.34917 × 10⁻¹0 + 5.19164 × 10⁻¹²·T³); T in K, temp range
                              285.0–645.0 K (Cox vapor pressure eq., Chao et al. 1983)
                              328 (extrapolated-Antoine eq., Boublík et al. 1984)
                              log (P/kPa) = 6.11997 – 1529.684/(206.648 + t°C); temp range 81.146–166.2°C (Antoine eq. from reported
                              exptl. data Forziati et al. 1949, Boublík et al. 1984)
                              330 (extrapolated-Antoine eq, Dean 1985, 1992)
                              log (P/mmHg) = 7.00314 – 1535.374/(207.30 + t°C); temp range 48–194°C (Antoine eq., Dean 1985, 1992)
                              log (P/kPa) = 6.1129 – 1532.449/(–66.123 + T/K); temp range 353–443 K (liquid, Antoine eq., Stephenson &
                              Malanowski 1987)
                              log (P/mmHg) = 15.1142 – 2.9821 × 10⁻³/(T/K) – 1.2619·log (T/K) – 6.3248 × 10⁻¹(T/K) + 3.5155 × 10⁻⁶·(T/K)²,
                              temp range 192–651 K (Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°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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<td>(20°C, selected from literature experimentally measured data, Staudinger &amp; Roberts 1996)</td>
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ln \[ \frac{H}{(atm \ m^3/mol)} \] = 5.557 – 3179/(T/K); temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)

Octanol/Water Partition Coefficient, log \( K_{ow} \):

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Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{oc} \):

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO₃ radical and \( k_{O_3} \) with O₃ or as indicated, *data at other temperatures see reference:

\[
k_{OH} = (8.2 \pm 1.6) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at } 305 \pm 2 \text{ K (relative rate method, Lloyd et al. 1976)}
\]

\[
k_{OH} = 8.2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \text{ at half-life of } 0.24–2.4 \text{ h (Darnall et al. 1976)}
\]

\[
k_{OH} = 12.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at room temp. (Atkinson 1985)}
\]

\[
k_{OH} = 12.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (relative rate method, Ohta & Ohyama 1985)}
\]

\[
k_{OH} = 12.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (recommended, Atkinson 1989, 1990)}
\]

\[
k_{OH}(\text{calc}) = 17.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ (molecular orbital calculations, Klamt 1993)}
\]

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration

Half-Lives in the Environment:

Air: \( t_{1/2} = 0.24–2.4 \text{ h} \), based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al. 1976; Howard et al. 1991); summer daylight lifetime \( \tau = 11 \text{ h} \) due to reaction with OH radical (Altshuller 1991).

Surface water: \( t_{1/2} = 0.5 \text{ d} \) 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 \( \text{o-ethyltoluene} \) at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C\cdot\log (T/K)
\end{align*}
\]

\( (1) \) \hspace{1cm} \( (1a) \) \hspace{1cm} \( (2) \) \hspace{1cm} \( (2a) \) \hspace{1cm} \( (3) \) \hspace{1cm} \( (4) \)

- Stull 1947
- Forziati et al. 1949
- Zwolinski & Wilhoit 1971

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- eq. 2
- \( \Delta H_f/(kJ \text{ mol}^{-1}) = \)

### FIGURE 3.1.1.12.1
Logarithm of vapor pressure versus reciprocal temperature for 1-ethyl-2-methylbenzene (o-ethyltoluene).
### 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:** C₉H₁₂, C₆H₄CH₃C₂H₅
- **Molecular Weight:** 120.191
- **Melting Point (°C):** –95.6 (Lide 2003)
- **Boiling Point (°C):**
  - 161.3 (Forziati et al. 1949, Weast 1982–83; Lide 2003)
- **Density (g/cm³):**
  - 0.8645 (20°C, Weast 1982–83)
- **Molar Volume (cm³/mol):**
  - 139.0 (20°C, calculated-density)
  - 162.6 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Fusion, ∆Hₘₚ (kJ/mol):**
- **Entropy of Fusion ∆Sₘₚ (J/mol K):**
- **Fugacity Ratio at 25°C, F:** 1.0
- **Water Solubility (g/m³ or mg/L at 25°C):**
- **Vapor Pressure (Pa at 25°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* (32.3°C, summary of literature data, temp range 7.2–161.3°C, Stull 1947)
  - 3066* (62.1°C, mercury manometer, measured range 62.1–160.3°C, Buck et al. 1949)
  - 6417* (78.105°C, ebulliometry, measured range 78.105–154.053°C, Forziati et al. 1949)
  - log (P/mmHg) = 7.01582 – 1529.784/(208.509 + t/°C); temp range 78.1–162.3°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
  - 399 (extrapolated-Antoine eq., Dreisbach 1955)
  - log (P/mmHg) = 7.01582 – 1529.184/(208.51 + t/°C); temp range 46–190°C (Antoine eq., Dean 1985, 1992)
  - log (P/mmHg) = 39.8909 – 3.6042 × 10³/(T/K) – 11.466·log (T/K) + 3.5274 × 10⁻²·(T/K) + 7.3492 × 10⁻¹⁴·(T/K)², temp range 178–637 K (Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log \( K_{OW} \):
- 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 \( K_{OA} \):

Bioconcentration Factor, log \( BCF \) or log \( K_B \):

Sorption Partition Coefficient, log \( K_{OC} \):
- 2.42 (aquifer material with \( f_{OC} \) of 0.006 and measured partition coeff. \( K_p = 1.58 \text{ mL/g.} \), Abdul et al. 1990)

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Volatileization:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO_3 radical and \( k_{O_3} \) with \( O_3 \) or as indicated, *data at other temperatures see reference:
- \( k_{OH} = (11.7 \pm 2.3) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \) at 305 ± K (relative rate method, Lloyd et al. 1976)
- \( k_{OH} = 11.7 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1} \) with estimated \( t_{1/2} \sim 0.24–2.4 \text{ h} \) (Darnall et al. 1976)
- \( k_{OH} = (21.3 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at room temp. (relative rate method, Ohta & Ohyama 1985; Atkinson 1989)
- \( k_{OH} = 1.92 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K (recommended, Atkinson 1989, 1990)
- \( k_{OH} \text{(calc)} = 20.93 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) (molecular orbital calculations, Klamt 1993)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (\( k_1 \) and \( k_2 \)):

Half-Lives in the Environment:
- Air: \( t_{1/2} = 0.24–2.4 \text{ h} \), based on rate of disappearance for the reaction with hydroxyl radical (Darnall et al 1976; Howard et al. 1991); summer daylight lifetime \( \tau = 7.2 \text{ h} \) due to reaction with OH radical (Altshuller 1991).
TABLE 3.1.13.1
Reported vapor pressures of \textit{m}-ethyltoluene at various temperatures and the coefficients for the vapor pressure equations

\begin{align*}
\log P &= A - B/(T/K) \\
\ln P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\ln P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C\log (T/K)
\end{align*}

Stull 1947 \quad \text{(1)} \quad \text{(1a)} \quad \text{(2)} \quad \text{(2a)} \quad \text{(3)} \quad \text{(4)}

| \text{reported vapor pressures} & \text{Forziati et al. 1949} & \text{Buck et al. 1949} & \text{Zwolinski & Wilhoit 1971} |
|-----------------------------|-----------------|-----------------|--------------------------|
| \text{summary of literature data} | \text{ebulliometry} | \text{mercury manometer} | \text{selected values} |
| \text{t/°C} | \text{P/Pa} | \text{t/°C} | \text{P/Pa} | \text{t/°C} | \text{P/Pa} | \text{t/°C} | \text{P/Pa} |
| 7.2 | 133.3 | 78.105 | 6417 | 62.1 | 3066 | 45.68 | 1333 |
| 32.3 | 666.6 | 82.525 | 7697 | 74 | 5386 | 59.07 | 2666 |
| 44.7 | 1333 | 86.293 | 8993 | 77.9 | 6293 | 67.58 | 4000 |
| 58.2 | 2666 | 89.793 | 10328 | 85.4 | 8693 | 73.95 | 5333 |
| 73.3 | 5333 | 93.022 | 11720 | 91.3 | 10879 | 79.102 | 6666 |
| 82.9 | 7999 | 97.368 | 13840 | 95.1 | 12772 | 83.45 | 7999 |
| 95.9 | 13332 | 102.36 | 16641 | 102.1 | 16772 | 90.584 | 10666 |
| 115.5 | 26664 | 107.38 | 19944 | 115.3 | 26398 | 96.363 | 13332 |
| 137.8 | 53329 | 112.07 | 23473 | 122.5 | 34264 | 107.456 | 19998 |
| 161.3 | 101325 | 118.33 | 28978 | 129.8 | 42397 | 115.829 | 26664 |
| \text{mp/°C} | –104.7 | 124.08 | 34920 | 140.7 | 58262 | 122.635 | 33331 |
| 131.027 | 43351 | 148.5 | 72527 | 128.412 | 39997 |
| 138.178 | 53692 | 160.3 | 99592 | 137.949 | 53329 |
| 145.795 | 66792 | \text{eq. 2} P/mmHg | A \quad 7.01582 | \text{eq. 2} P/mmHg | A \quad 7.01582 |
| 154.053 | 83749 | B \quad 1529.184 | C \quad 5.663 | B \quad 1529.184 |
| \text{bp/°C} | 161.305 | \text{bp/°C} | 161.305 | \text{bp/°C} | 161.305 |
| \text{∆H_v/(kJ mol}^{-1}) | \text{at 25°C} | 46.9 | \text{at bp} | 38.53 |

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FIGURE 3.1.13.1 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: C₉H₁₂, C₆H₄CH₃C₂H₅
Molecular Weight: 120.191
Melting Point (°C):
–62.35 (Lide 2003)
Boiling Point (°C):
162 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
0.8614 (Weast 1982–83)
Molar Volume (cm³/mol):
139.5 (20°C, calculated density, Stephenson & Malanowski 1987)
162.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ∆Hₘₚ (kJ/mol):
Entropy of Fusion ∆Sₘₚ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
40.0 (estimated from nomograph, Kabadi & Danner 1979)
94.85 (shake flask-GC, Mackay & Shiu 1981)
Vapor Pressure (Pa at 25°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* (32.7°C, summary of literature data, temp range 7.6–162°C, Stull 1947)
3840* (66.8°C, mercury manometer, measured range 66.8–161.1°C, Buck et al. 1949)
6417* (78.396°C, ebulliometry, measured range 78.396–154.684°C, Forziati et al. 1949)
log (P/mmHg) = 6.99801 – 1527.113/(208.921 + t/°C); temp range 78.3–163.0°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
402 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 6.99802 – 1527.113/(208.921 + t/°C); temp range 65–210°C (Antoine eq. for liquid state, Dreisbach 1955)
393* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.99802 – 1527.113/(208.921 + t/°C); temp range 45.68–191.0°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 10461.1/(T/K)] + 8.175267; temp range 7.6–162°C (Antoine eq., Weast 1972–73)
log (P/atm) = (1 – 345.228/T) × 10^4(0.856105 – 6.18307 × 10^4·T + 5.08568 × 10^7·T²); 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 (P/mmHg) = 6.99802 – 1527.113/(208.921 + t/°C); temp range 46–191°C (Antoine eq., Dean 1985, 1992)
log (P/kPa) = 6.11098 – 1519.486/(–65.035 + T/K); temp range 349–442 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 46.9026 – 3.8382 × 10³/(T/K) – 14.154·log (T/K) + 4.9305 × 10⁻³·(T/K) – 1.3901 × 10⁻¹³·(T/K)²; temp range 211–640 K (Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):

498  (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log $K_{OW}$:

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 $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO₃ radical and $k_{O3}$ with O₃ or as indicated, *data at other temperatures see reference: $k_{OH} = (7.8 \pm 1.6) \times 10^9$ L mol⁻¹ s⁻¹ at 305 ± 2 K (relative rate method, Lloyd et al. 1976)
$k_{OH} = 7.8 \times 10^9$ L mol⁻¹ s⁻¹ with $t_{1/2} = 0.24–2.4$ h (Darnall et al. 1976)
$k_{OH} = 12.9 \times 10^{-12}$ cm³ molecule⁻¹ 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)
$k_{OH} = 11.3 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Atkinson 1985)
$k_{OH} = 12.8 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (relative rate method, Ohta & Ohyama 1985)
$k_{OH} = 12.1 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ at 298 K (recommended, Atkinson 1989, 1990)
$k_{OH}(calc) = 21.6 \times 10^{-12}$ cm³ molecule⁻¹ s⁻¹ (molecular orbital calculations, Klamt 1993)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24–2.4$ 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 $\tau = 11$ 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(t/°C) \quad (2) \\
\log P &= A - B/(C + t/°C) \quad (3) \\
\log P &= A - B/(C + T/K) \quad (4) \\
\end{align*}
\]

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<td>t/°C</td>
<td>P/Pa</td>
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<td>146.368</td>
<td>66792</td>
</tr>
<tr>
<td>154.684</td>
<td>83750</td>
<td>eq. 2</td>
<td>P/mmHg</td>
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<td>A</td>
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<td>A</td>
<td>21.27</td>
</tr>
<tr>
<td>B</td>
<td>1527.113</td>
<td>B</td>
<td>2939</td>
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<tr>
<td>C</td>
<td>208.921</td>
<td>C</td>
<td>4.406</td>
</tr>
<tr>
<td>bp/°C</td>
<td>161.989</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \Delta H_v/(kJ \ \text{mol}^{-1}) = \]

at 25°C \[ 46.61 \]

at bp \[ 38.41 \]

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**FIGURE 3.1.14.1** 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: C_{10}H_{14}, CH_{3}C_{6}H_{4}CH(CH_{3})_{2}
Molecular Weight: 134.218
Melting Point (°C):
-67.94 (Lide 2003)
Boiling Point (°C):
177.1 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
0.8573 (Weast 1982–83)
Molar Volume (cm³/mol):
156.6 (20°C, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
9.66 (Dreisbach 1955)
9.67 (Chickos et al. 1999)
Entropy of Fusion ΔS_{fus} (J/mol K):
47.33, 46.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
34.15 (residue volume method, Booth & Everson 1948)
23.35 (shake flask-LSC, Banerjee et al. 1980)
50.7 ± 2.3 (shake flask-HPLC/UV, Lun et al. 1997)
Vapor Pressure (Pa at 25°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* (13.3°C, mercury manometer, Linder 1931)
log (P/mmHg) = 8.063 – 10670/(T/K) (isoteniscope method, measured range not specified, Kobe et al. 1941)
133.3* (19°C, summary of literature data, Stull 1947)
212 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 6.9260 – 1538.00/(203.10 + t/°C); temp range 80–215°C (Antoine eq. for liquid state, Dreisbach 1955)
12026* (107.04°C, ebulliometry, measured range107.04–178.42°C, McDonald et al. 1959)
204* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.9237 – 1537.06/(203.05 + t/°C); temp range 56.4–207.1°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/atm) = (1 – 450.311/T) × 10^((0.875129 – 6.86627 × 10^2·T + 5.61507 × 10^2·T^2); T in K, temp range 290.0–650.0 K (Cox vapor pressure eq., Chao et al. 1983)
log (P/mmHg) = 7.05074 – 1608.91/(208.72 + t/°C); temp range 107–178°C (Antoine eq., Dean 1985, 1992)
194 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.16214 – 1599.29/(–65.492 + T/K); temp range 380–452 K (liquid, Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = –5.5137 – 3.0256 × 10^(1·/(T/K)) + 8.9840·log (T/K) – 2.5597 × 10^–2·(T/K)^2 + 1.3823 × 10^–5·(T/K)^2, temp range 205–653 K (Yaws 1994)
Mononuclear Aromatic Hydrocarbons

Henry’s Law Constant (Pa m³/mol at 25°C):

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<th>Source</th>
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<tr>
<td>800</td>
<td>(calculated-P/C, Mackay &amp; Shiu 1981)</td>
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<tr>
<td>942</td>
<td>(computed-expert system SPARC, Kollig 1995)</td>
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Octanol/Water Partition Coefficient, log $K_{ow}$:

<table>
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<th>Value</th>
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<td>4.10</td>
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<td>3.45</td>
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<td>4.0</td>
<td>(computed-expert system SPARC, Kollig 1995)</td>
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Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

<table>
<thead>
<tr>
<th>Value</th>
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<td>3.70</td>
<td>(computed-$K_{OC}$, Kollig 1995)</td>
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</table>

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatilization:

Photolysis: rate constant of $1.68 \times 10^{-2}$ h⁻¹ with H₂O₂ under photolysis at 25°C in F-113 solution and with HO• in the gas (Dilling et al. 1988).

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO₃ radical and $k_{O3}$ with O₃ or as indicated, *data at other temperatures see reference:

$\text{k_{OH}} = 0.92 \times 10^{11}$ M⁻¹ s⁻¹ at room temp. (estimated from structurally similar p-ethyltoluene, Winer et al. 1976)

$\text{k_{OH}(calc)} = 1.50 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at room temp. (SAR, Atkinson 1987)

$\text{k_{OH}} = 1.53 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ at room temp. (Dilling et al. 1988)

$\text{k_{OH}} = (1.51 \pm 0.41) \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹ with a tropospheric lifetime $\tau = 1.0-1.4$ d; $\text{k_{NO3}} = (9.9 \pm 1.6) \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹ with a tropospheric lifetime $\tau = 1.3$ yr and a calculated tropospheric lifetime $\tau > 330$ d due to reaction with O₃ at 295 ± 2 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 d and 1.3 yr due to reactions with OH radical, O₃ and NO₃ radical, respectively (Corchnoy & Atkinson 1990)
TABLE 3.1.15.1
Reported vapor pressures of \( p \)-cymene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\text{log } P &= A - B/(T/K) \quad (1) \\
\text{log } P &= A - B/(C + t/°C) \quad (2) \\
\text{log } P &= A - B/(C + T/K) \quad (3) \\
\text{log } P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

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<td>101325</td>
<td>A</td>
<td>7.03724</td>
</tr>
<tr>
<td>B</td>
<td>1599.29</td>
<td>136.5</td>
<td>33331</td>
</tr>
<tr>
<td>C</td>
<td>207.659</td>
<td>142.6</td>
<td>39997</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–67.98</td>
<td>152.6</td>
<td>53329</td>
</tr>
<tr>
<td>Kobe et al. 1941</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>isoteniscope method</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>data presented by</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
eq 1 P/mmHg |
| A | 8.063 |
| B | 2332 |
| bp/°C | 176.8 |
| \( \Delta H_v/(kJ \text{ mol}^{-1}) = 44.64 \) |
| eq. 2 P/mmHg |
| A | 6.9237 |
| B | 1537.06 |
| C | 203.05 |
| bp/°C | 177.13 |
| \( \Delta H_v/(kJ \text{ mol}^{-1}) = \) |
| at 25°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: \( C_{10}H_{14}, C_6H_5(CH_2)_3CH_3 \)

Molecular Weight: 134.218

Melting Point (°C):

\(-87.85 \quad \text{(Lide 2003)}\)

Boiling Point (°C):

183.31 \quad \text{(Lide 2003)}

Density (g/cm\(^3\) at 20°C):

0.8601 \quad \text{(Weast 1982–83)}

Molar Volume (cm\(^3\)/mol):

156.1 \quad \text{(20°C, calculated-density)}

184.8 \quad \text{(calculated-Le Bas method at normal boiling point)}

Enthalpy of Fusion \( \Delta H_{\text{fus}} \) (kJ/mol):

10.98 \quad \text{(Dreisbach 1955)}

11.22 \quad \text{(Chickos et al. 1999)}

Entropy of Fusion \( \Delta S_{\text{fus}} \) (J/mol K):

60.56, 66.5 \quad \text{(exptl., calculated-group additivity method, Chickos et al. 1999)}

Fugacity Ratio at 25°C, \( F \): 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°C; *data at other temperatures are tabulated at end of section):

12.6 \quad \text{(shake flask-UV, Andrews & Keefer 1950)}

50.5 \quad \text{(shake flask-UV, Klevens 1950)}

15.4 \quad \text{(estimated, Deno & Berkheimer 1960)}

17.7 \quad \text{(shake flask-GC/ECD, Massaldi & King 1973)}

11.8 \quad \text{(shake flask-GC, Sutton & Calder 1975)}

12.6 \quad \text{(shake flask-GC, Mackay & Shiu 1981)}

13.83 \quad \text{(generator column-HPLC/UV, GC/ECD, Tewari et al. 1982)}

13.8 \quad \text{(generator column-HPLC/UV, Wasik et al. 1983)}

13.76* \quad \text{(generator column-HPLC/UV, measured range 7–45°C, Owens et al. 1986)}

15.0 \quad \text{(IUPAC recommended, Shaw 1989b)}

16.7* \quad \text{(30°C, equilibrium flow cell-GC, measured range 30–100°C, Chen & Wagner 1994c)}

\ln x = -43.2390 - 5720.35/(T/K) - 1.221 \times 10^{-4} \cdot (T/K)^2; \text{ temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)}

12.25* \quad \text{(vapor absorption technique-HPLC/UV, measured range 0.5–55°C, Dohányosová et al. 2001)}

\ln x = -346.295 + 14524.83/(T/K) + 49.9130 \cdot \ln (T/K); \text{ temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)}

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations; *data at other temperatures are tabulated at end of section):

64* \quad \text{(12.2°C, mercury manometer, Linder 1931)}

133.3* \quad \text{(22.7°C, summary of literature data, Stull 1947)}

6415* \quad \text{(96.233°C, ebulliometry, measured range 96.233–184.329°C, Forziati et al. 1949)}

\log (P/mmHg) = 6.98318 – 1577.965/(201.378 + t/°C); \text{ temp range 96.2–184.2°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)}

145 \quad \text{(extrapolated-Antoine eq., Dreisbach 1955)}

\log (P/mmHg) = 6.98317 – 1577.965/(201.378 + t/°C); \text{ temp range 85–220°C (Antoine eq. for liquid state, Dreisbach 1955)}
Mononuclear Aromatic Hydrocarbons

\[ \log(P/\text{mmHg}) = 6.98317 - \frac{1577.965}{201.378 + t/\degree C}; \text{ temp range 62.36–213.1\degree C (Antoine eq., Zwolinski & Wilhoit 1971)} \]

\[ \log(P/\text{mmHg}) = \left[ -0.2185 \times 11052.1/(T/K) \right] + 8.194170; \text{ temp range 22.7–183.1\degree C (Antoine eq., Weast 1972–73)} \]

\[ \log(P/\text{atm}) = (1 - 456.368/T) \times 10^{0.889482 - 7.01171 \times 10^4 \cdot T + 5.65027 \times 10^7 \cdot T^2}; T \text{ in K, temp range 295.0–660.0 K (Cox vapor pressure eq., Chao et al. 1983)} \]

\[ \log(P/\text{kPa}) = 6.11624 - 1583.708/(202.013 + t/\degree C); \text{ temp range 96.2–184.3\degree C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]

\[ \log(P/\text{kPa}) = 6.22353 - 1660.274/(210.314 + t/\degree C); \text{ temp range 101.3–181.8\degree C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]

\[ \log(P/\text{mmHg}) = 6.98317 - \frac{1577.965}{201.378 + t/\degree C}; \text{ temp range 62–213\degree C (Antoine eq., Dean 1985, 1992)} \]

\[ \log(P_L/\text{kPa}) = 6.09809 - \frac{1571.648}{–72.413 + T/K}; \text{ temp range: 369–463 K (Antoine eq., Stephenson & Malanowski 1987)} \]

\[ 110 \quad (20.51\degree C, \text{ static method, measured range 243.8–403.14 K, Kasehgari et al. 1993}) \]

\[ \log(P/\text{kPa}) = 6.41845 - 1779.018/(220.982 + t/\degree C); \text{ temp range 243.8–403.14 K (static method, Kasehgari et al. 1993)} \]

\[ \log(P/\text{mmHg}) = 49.9687 - 4.3981 \times 10^5/(T/K) - 14.352 \log (T/K) + 4.2054 \times 10^{-11} \cdot (T/K) + 3.4379 \times 10^{-6} \cdot (T/K)^2, \text{ temp range 185–661 K (Yaws 1994)} \]

\[ 107 \quad (20.16\degree C, \text{ static method, measured range 253.76–418.04 K, Mokbel et al. 1998}) \]

Henry’s Law Constant (Pa m^3/mol at 25\degree C; *data at other temperatures are tabulated at end of section):

1300 \quad (\text{calculated-P/C, Mackay & Shiu 1981})

1332 \quad (\text{calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991})

1502 \quad (\text{infinite activity coeff. } \gamma^\infty \text{ in water determined by inert gas stripping-GC, Li et al. 1993})

1692* \quad (\text{equilibrium headspace-GC, Perlinger et al. 1993})

1357.8 \quad (\text{modified EPICS method-GC, Ryu & Park 1999})

Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):

4.26 \quad (\text{Hansch & Leo 1979})

4.19 \quad (\text{calculated-fragment const., Rekker 1977})

3.86 \quad (\text{headspace GC, Hutchinson et al. 1980})

4.26 \quad (\text{HPLC-k’ correlation, Hammers et al. 1982})

4.28 \quad (\text{generator column-HPLC/UV, Tewari et al. 1982c})

4.21 \quad (\text{HPLC methods, Harnisch et al. 1983})

4.28 \quad (\text{generator column-HPLC/UV, Wasik et al. 1983})

4.29 \quad (\text{generator column-RP- LC, Schantz & Martire 1987})

4.26, 4.50 \quad (\text{RP-HPLC-k’ correlations, Sherblom & Eganhouse 1988})

4.26 \quad (\text{recommended, Sangster 1989, 1993})

4.377 \quad (\text{shake flask/slow stirring-GC, De Brujin et al. 1989})

4.38 \quad (\text{recommended, Hansch et al. 1995})

Bioconcentration Factor, log \(B_{\text{CF}}\):

Sorption Partition Coefficient, log \(K_{\text{oc}}\):

3.39 \quad (\text{average 5 soils and 3 sediments, sorption isotherms by batch equilibrium and column experiments, Schwarzenbach & Westall 1981})

3.40 \quad (\text{sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987})

3.52 \quad (\text{RP-HPLC-k’ correlation, cyanopropyl column, Hodson & Williams 1988})

3.15, 3.32 \quad (\text{RP-HPLC-k’ correlation, Szabo et al. 1990a,b})

3.35, 3.38, 3.39 \quad (\text{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 \textit{n}-butylbenzene at various temperatures

<table>
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<tr>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
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<tr>
<td>7</td>
<td>13.34</td>
<td>30</td>
<td>16.7</td>
<td>0.5</td>
<td>11.5</td>
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<td>10</td>
<td>12.98</td>
<td>40</td>
<td>17.82</td>
<td>5</td>
<td>11.5</td>
<td>15</td>
<td>828</td>
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<tr>
<td>12.5</td>
<td>13.14</td>
<td>50</td>
<td>20.3</td>
<td>15</td>
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<td>60</td>
<td>26.9</td>
<td>25</td>
<td>12.25</td>
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<tr>
<td>17.5</td>
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<td>14.5</td>
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<td>2168</td>
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<td>13.66</td>
<td>80</td>
<td>47.72</td>
<td>45</td>
<td>17.6</td>
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<td></td>
</tr>
<tr>
<td>25</td>
<td>13.76</td>
<td>90</td>
<td>61.14</td>
<td>55</td>
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<tr>
<td>30</td>
<td>14.58</td>
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<td>83.5</td>
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<tr>
<td>35</td>
<td>15.4</td>
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<tr>
<td>40</td>
<td>1763</td>
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<td></td>
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<td>1.29</td>
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</tr>
<tr>
<td>45</td>
<td>20.21</td>
<td></td>
<td></td>
<td></td>
<td>6.60 at 25°C</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 1.29 \]

\[ \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 6.60 \text{ at 25°C} \]

### FIGURE 3.1.1.16.1
Logarithm of mole fraction solubility and Henry's law constant versus reciprocal temperature for \textit{n}-butylbenzene.
### TABLE 3.1.16.2

Reported vapor pressures of *n*-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \\
\log P = A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\]

<table>
<thead>
<tr>
<th>Temperature/°C</th>
<th>Linder 1931</th>
<th>Forziati et al. 1949</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mercury manometer</td>
<td>summary of literature data</td>
<td>ebulliometry</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>0.47</td>
<td>13.3</td>
<td>22.7</td>
<td>133.3</td>
</tr>
<tr>
<td>5.5</td>
<td>33.3</td>
<td>48.8</td>
<td>666.6</td>
</tr>
<tr>
<td>12.2</td>
<td>64</td>
<td>63</td>
<td>1333</td>
</tr>
<tr>
<td></td>
<td></td>
<td>76.3</td>
<td>2666</td>
</tr>
<tr>
<td></td>
<td></td>
<td>92.4</td>
<td>5333</td>
</tr>
<tr>
<td></td>
<td></td>
<td>102.6</td>
<td>7999</td>
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<td>116.2</td>
<td>13332</td>
</tr>
<tr>
<td></td>
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<td>136.9</td>
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<tr>
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<td>159.2</td>
<td>53329</td>
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<tr>
<td>183.1</td>
<td>101325</td>
<td>151.541</td>
<td>43352</td>
</tr>
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<td>182.4</td>
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<td>159.032</td>
<td>53693</td>
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<td>181.7</td>
<td>97645</td>
<td>175.666</td>
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</tr>
<tr>
<td>180.4</td>
<td>97645</td>
<td>172.91</td>
<td>79993</td>
</tr>
<tr>
<td>179.9</td>
<td>93226</td>
<td>181.767</td>
<td>97645</td>
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<tr>
<td>179.5</td>
<td>93226</td>
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<td>179.1</td>
<td>85992</td>
<td>183.636</td>
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<td>178.7</td>
<td>85992</td>
<td>183.725</td>
<td>102456</td>
</tr>
<tr>
<td>178.3</td>
<td>85992</td>
<td>184.329</td>
<td>103989</td>
</tr>
</tbody>
</table>

eq. 2 \[ \frac{P}{mmHg} \]

| A | 698318 |
| B | 1577.965 |
| C | 201.378 |

bp/°C 183.27

\[ \Delta H_v/(kJ \ mol^{-1}) \]

at 25°C 50.12

at bp 37.75

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FIGURE 3.1.16.2 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: C_{10}H_{14}, C_6H_5CH_2CH(CH_3)_2
Molecular Weight: 134.218
Melting Point (°C):
-51.4  (Lide 2003)
Boiling Point (°C):
170.5  (Stephenson & Malanowski 1987)
Density (g/cm³ at 20°C):
0.8532  (Weast 1982–83)
Molar Volume (cm³/mol):
157.3  (20°C, calculated-density)
184.8  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_fus (kJ/mol):
12.51  (Dreisbach 1955)
Entropy of Fusion ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
10.1  (shake flask-GC, Price 1976)
Vapor Pressure (Pa at 25°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°C, summary of literature data, Stull 1947)
6415*  (86.637°C, ebulliometry, measured range 86.637–173.814°C, Forziati et al. 1949)
log (P/mmHg) = 6.93033 – 1526.384/(204.171 + t/°C); temp range 86.6–173.8°C (manometer, Antoine eq. from exptl. data, Forziati et al. 1949)
257  (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 6.93033 – 1526.384/(204.171 + t/°C); temp range 75–210°C (Antoine eq. for liquid state, Dreisbach 1955)
248*  (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.92804 – 1525.446/(204.122 + t/°C); temp range 53.21–202.45°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [–0.2185 × 8567.8/(T/K)] + 7.048112; temp range: –9.8 to 170.5°C (Antoine eq., Weast 1972–73)
log (P/atm) = (1 – 445.940/T) × 10^(0.870338 – 6.75481 × 10⁴·T + 5.59009 × 10⁷·T²); 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 (P/kPa) = 6.06156 – 1530.811/(204.675 + t/°C); temp range 86.64–173.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
log (P/T·kPa) = 6.06898 – 1536.514/(-67.788 + T/K); temp range 373–447 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = –7.0438 – 2.6892 × 10¹/(T/K) + 8.7843·log (T/K) – 2.1426 × 10⁻²·(T/K) + 1.1248 × 10⁻⁵·(T/K)²; temp range 222–650 K (Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°C):
1160, 1714  (calculated-CW/CA, calculated-bond contribution, Hine & Mookerjee 1975)
3300  (calculated-P/C, Mackay & Shiu 1981)
1393  (calculated-QSAR, Nirmalakhandan & Speece 1988b)
Octanol/Water Partition Coefficient, log $K_{OW}$:
- 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 $K_{OC}$:

Environmental Fate Rate Constants or Half-Lives:
- Volatilization: estimated $t_{1/2} \sim 3.2$ h, evaporation from a river of 1 m depth with wind speed 3 m/s and water current of 1 m/s at 20°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

<table>
<thead>
<tr>
<th>Summary of literature data</th>
<th>Forziati et al. 1949</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>P/Pa</td>
<td>$t/°C$</td>
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<td>-----</td>
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</tr>
<tr>
<td>-9.8</td>
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<td>P/mmHg</td>
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<td>bp/°C</td>
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<tr>
<td></td>
<td>$\Delta H_v/(kJ \text{ mol}^{-1})$=</td>
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<td>$bp/°C$</td>
<td>172.759</td>
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FIGURE 3.1.17.1 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: C_{10}H_{14}, C_6H_5CH(CH_3)C_2H_5
Molecular Weight: 134.218
Melting Point (°C): -82.7 (Lide 2003)
Boiling Point (°C): 173.3 (Lide 2003)
Density (g/cm³ at 20°C): 0.8621 (Weast 1982–83)
Molar Volume (cm³/mol):
155.7 (20°C, calculated from density)
184.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
9.83 (Dreisbach 1955)
Entropy of Fusion ΔS_{fus} (J/mol K):

Water Solubility (g/m³ or mg/L at 25°C):
30.9 (shake flask-UV, Andrews & Keefer 1950)
17.6 (shake flask-GC, Sutton & Calder 1975)
Vapor Pressure (Pa at 25°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* (9.8°C, mercury manometer, measured range –8.6 to 9.8°C, Linder 1931)
133.3* (18.6°C, summary of literature data, temp range 18.6–175.3°C, Stull 1947)
6415* (87.118°C, ebulliometry, measured range 87.118–174.358°C, Forziati et al. 1949)
\log (P/mmHg) = 6.95097 – 1540.174/(205.101 + t°C); temp range 87.1–174.4°C, (manometer, Antoine eq. from expltl. data, Forziati et al. 1949)
250 (extrapolated, Antoine eq., Dreisbach 1955)
\log (P/mmHg) = 6.95097 – 1540.174/(205.101 + t°C); temp range 75–210°C (Antoine eq. for liquid state, Dreisbach 1955)
241* (extrapolated, Antoine eq., Zwolinski & Wilhoit 1971)
\log (P/mmHg) = 6.94866 – 1539.233/(205.052 + t°C); temp range 53.7–202.95°C (Antoine eq., Zwolinski & Wilhoit 1971)
\log (P/mmHg) = [-0.2185 × 11609.3/(T/K)] + 8.318014; temp range 18.6–175.3°C (Antoine eq., Weast 1972–73)
\log (P/atm) = (1 – 446.499/T) × 10^8(0.870844 – 6.72060 × 10^3T + 5.52698 × 10^7T^2); T in K, temp range 258.0–645.0 K (Cox vapor pressure eq., Chao et al. 1983)
240 (extrapolated, Antoine eq., Boublik et al. 1984)
\log (P/mmHg) = 6.05072 – 1533.897/(204.382 + t°C); temp range 87.12–174.4°C (Antoine eq. from reported expltl. data, Boublik et al. 1984)
\log (P/mmHg) = 6.94219 – 1533.95/(204.39 + t°C); temp range 87–174°C (Antoine eq., Dean 1985. 1992)
\log (P/kPa) = 6.10298 – 1559.452/(C + T/K); temp range 384–448 K (Antoine eq., Stephenson & Malanowski 1987)
\log (P/kPa) = 6.47915 – 1781.723/(208.35 + t°C); temp range 243.92–373.39 K (static method, Kasehgari et al. 1993)
Mononuclear Aromatic Hydrocarbons

\[ \log \left( \frac{P}{\text{mmHg}} \right) = 61.5904 - 4.5093 \times 10^3/(T/K) - 19.522 \log (T/K) + 6.9865 \times 10^{-3} (T/K) + 7.8205 \times 10^{-14} (T/K)^2, \]
\text{temp range 198–665 K (Yaws 1994)}

186* \quad (20.23^\circ \text{C}, \text{static method, measured range 263.52–393.39 K, Mokbel et al. 1998})

Henry’s Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 4.44, 4.70 \quad \text{(RP-HPLC-}k’\text{ correlations, Sherblom & Eganhouse 1988)}
- 4.57 \quad \text{(average lit. value, Sangster 1993)}
- 4.44 \quad \text{(Hansch et al. 1995)}
- 3.90 \quad \text{(computed-expert system SPARC, Kollig 1995)}

Octanol/Air Partition Coefficient, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):

Sorption Partition Coefficient, \( \log K_{OC} \):
- 2.71 \quad \text{(aquifer material with f}_{OC}\text{ of 0.006 and measured partition coeff. } K_P = 3.06 \text{ mL/g., Abdul et al. 1990)}
- 3.60 \quad \text{(computed-K}_{OW}\text{, Kollig 1995)}

Environmental Fate Rate Constants or Half-Lives:

Half-Lives in the Environment:

### TABLE 3.1.1.18.1

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<th>Temperature (°C)</th>
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### TABLE 3.1.1.18.1 (Continued)

#### 1.

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$\text{data fitted to Wagner eq.}$

Antoine eq.

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**FIGURE 3.1.18.1** 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, tert-butylbenzene
Chemical Name: tert-butylbenzene
CAS Registry No: 98-06-6
Molecular Formula: C_{10}H_{14}, C_6H_5C(CH_3)_3
Molecular Weight: 134.218
Melting Point (°C):
-58 (Stephenson & Malanowski 1987)
Boiling Point (°C):
169.1 (Lide 2003)
Density (g/cm³ at 20°C):
0.8665 (Weast 1982–83)
Molar Volume (cm³/mol):
154.9 (20°C, calculated from density)
184.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
8.38 (Dreisbach 1955)
8.40 (Chickos et al. 1999)
Entropy of Fusion ΔS_{fus} (J/mol K):
39.1, 45.4 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
34.0 (shake flask-UV, Andrews & Keefer 1950)
29.5 (shake flask-GC, Sutton & Calder 1975)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
144* (13.7°C, mercury manometer, measured range −2 to 13.7°C, Linder 1931)
133.3* (13°C, summary of literature data, temp range 13–168.5°C, Stull 1947)
6426* (83.887°C, ebulliometry, measured range 83.887–170.165°C, Forziati et al. 1949)
log (P/mmHg) = 9.2050 − 1504.572/(203.280 + t/°C); temp range 83.9–170.2°C (manometer, Antoine eq. from exp. data, Forziati et al. 1949)
295 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 6.92050 − 1504.572/(203.280 + t/°C); temp range 70–205°C (Antoine eq. for liquid state, Dreisbach 1955)
286* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 6.91829 − 1503.651/(203.280 + t/°C); temp range 50.79–198.54°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [−0.2185 × 10705.5/(T/K)] + 8.195269; temp range 13–168°C (Antoine eq., Weast 1972–73)
log (P/ atm) = (1 – 442.319/T) × 10^4(0.881530 − 7.21114 × 10^3T + 6.01764 × 10^7T^2); 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 (P/kPa) = 6.03861 − 1499.886/(202.792 + t/°C); temp range 83.88–170.2°C (Antoine eq. from reported exp. data of Forziati et al. 1949, Boublik et al. 1984)
286 (extrapolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 6.92255 − 1505.987/(203.49 + t/°C); temp range 84–170°C (Antoine eq., Dean 1985, 1992)
log (P_2/kPa) = 6.06067 – 1515.51/(–68.551 + T/K); temp range 368–444 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = 41.4522 – 3.9027 × 10^3/(T/K) – 11.410·log (T/K) + 2.4320 × 10^{-10}·(T/K) + 2.2517 × 10^{-6}·(T/K)^2,
temp range 215–660 K (Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
1200 (calculated-P/C, Mackay & Shiu 1981)
1300 (calculated-C_A/C_W, Eastcott et al. 1988)

Octanol/Water Partition Coefficient, log K_{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 K_{OA}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:
Volatilization/Evaporation:
Photolysis:
Oxidation: rate constant k = 4.58 × 10^{-12} cm^3 molecule^{-1} s^{-1} for the gas phase reaction with OH radical at room temp. (Ohta & Ohyama 1985; Atkinson 1989);
rate constant k = 4.6 × 10^{-12} cm^3 molecule^{-1} 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 3.1.19.1
Reported vapor pressures of tert-butylbenzene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\text{log } P &= A - B/(T/K) \quad (1) \\
\text{log } P &= A - B/(C + t/°C) \quad (2) \\
\text{log } P &= A - B/(C + T/K) \quad (3) \\
\text{log } P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

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<tr>
<th></th>
<th>Linder 1931</th>
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<th>Forziati et al. 1949</th>
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\[
\Delta H_v/(kJ \text{ mol}^{-1}) =
\begin{align*}
\text{at } 25°C & = 49.8 \\
\text{at bp} & = 37.61
\end{align*}
\]
**FIGURE 3.1.19.1** 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: \( C_{10}H_{14} \), \( C_6H_2(CH_3)_4 \)
Molecular Weight: 134.218
Melting Point (°C):
\[-6.2 \ (\text{Weast 1982–83; Lide 2003}) \]
Boiling Point (°C):
\[205 \ (\text{Weast 1982–83; Lide 2003}) \]
Density (g/cm\(^3\) at 20°C):
\[0.9052 \ (\text{Weast 1982–83}) \]
Molar Volume (cm\(^3\)/mol):
\[148.3 \ (20^\circ\text{C}, \text{calculated-density}) \]
\[184.8 \ (\text{calculated-Le Bas method at normal boiling point}) \]
Enthalpy of Fusion \( \Delta H_{\text{ fus}} \) (kJ/mol):
\[11.21 \ (\text{Dreisbach 1955}) \]
\[11.23 \ (\text{Chickos et al. 1999}) \]
Entropy of Fusion \( \Delta S_{\text{ fus}} \) (J/mol K):
\[42.31, 45.7 \ (\text{exptl., calculated-group additivity method, Chickos et al. 1999}) \]
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
\[133.3^* \ (42.6^\circ\text{C}, \text{summary of literature data, temp range 42.6–204.4^\circ\text{C}, Stull 1947}) \]
\[49.20 \ (\text{extrapolated-Antoine eq., Dreisbach 1955}) \]
\[\log (P/\text{mmHg}) = 7.0584 - 1689.10/(199.28 + t/\text{°C}); \text{ temp range 100–250^\circ\text{C}} \ (\text{Antoine eq. for liquid state, Dreisbach 1955}) \]
\[1333^* \ (79.515^\circ\text{C}, \text{compiled data, temp range 79.515–235.815^\circ\text{C}, Bond & Thodos 1960}) \]
\[45.01^* \ (\text{extrapolated-Antoine eq., Zwolinski & Wilhoit 1971}) \]
\[\log (P/\text{mmHg}) = 7.0594 - 1690.54/(199.48 + t/\text{°C}); \text{ temp range 79.5–235.69^\circ\text{C}} \ (\text{liquid, Antoine eq., Zwolinski & Wilhoit 1971}) \]
\[\log (P/\text{mmHg}) = -0.2185 \times 12258.0/(T/\text{K}) + 8.534237; \text{ temp range 42.6–204.4^\circ\text{C}} \ (\text{Antoine eq., Weast 1972–73}) \]
\[\log (P/\text{atm}) = (1 - 478.255/T) \times 10^4(0.889494 - 6.47585 \times 10^{-1}T + 4.96841 \times 10^{-2}T^2); \text{ T in K, temp range 310.0–690.0 K} \ (\text{Cox vapor pressure eq., Chao et al. 1983}) \]
\[45.01 \ (\text{extrapolated-Antoine eq., Dean 1985, 1992}) \]
\[\log (P/\text{mmHg}) = 7.0594 - 1690.54/(199.48 + t/\text{°C}); \text{ temp range 80–217^\circ\text{C}} \ (\text{Antoine eq., Dean 1985, 1992}) \]
\[45.02 \ (\text{extrapolated-Antoine eq., Stephenson & Malanowski 1987}) \]
\[\log (P/\text{kPa}) = 6.1843 - 1690.54/(–73.67 + T/K); \text{ temp range 352–509 K} \ (\text{liquid, Antoine eq., Stephenson & Malanowski 1987}) \]

Henry’s Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
\[3.84 \ (\text{generator column-HPLC, Wasik et al. 1982}) \]
\[4.11 \ (\text{HPLC-k correlation, Hammers et al. 1982}) \]

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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 $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

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

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
<th>Coefficients</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>42.6</td>
<td>133.3</td>
<td>log $P = A - B/(T/K)$</td>
<td>(1)</td>
</tr>
<tr>
<td>68.7</td>
<td>666.6</td>
<td>$\ln P = A - B/(T/K)$</td>
<td>(1a)</td>
</tr>
<tr>
<td>81.8</td>
<td>1333</td>
<td>$\log P = A - B/(C + t/°C)$</td>
<td>(2)</td>
</tr>
<tr>
<td>95.8</td>
<td>2666</td>
<td>$\log P = A - B/(C + T/K)$</td>
<td>(3)</td>
</tr>
<tr>
<td>111.5</td>
<td>5333</td>
<td>$\log P = A - B/(T/K) - C\cdot\log (T/K)$</td>
<td>(4)</td>
</tr>
<tr>
<td>121.8</td>
<td>7999</td>
<td>$\log P = A - B/(T/K) - C\cdot\log (T/K) + D\cdot P/(T/K)^2$</td>
<td>(5)</td>
</tr>
</tbody>
</table>

Stull 1947  
Bond & Thodos 1960  
Zwolinski & Wilhoit 1971

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>135.7</td>
<td>13332</td>
</tr>
<tr>
<td>1155.7</td>
<td>26664</td>
</tr>
<tr>
<td>180</td>
<td>53329</td>
</tr>
<tr>
<td>204.4</td>
<td>101325</td>
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</table>

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
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<td>$27.4323$</td>
</tr>
<tr>
<td>B</td>
<td>$3713.52$</td>
</tr>
<tr>
<td>C</td>
<td>$6774$</td>
</tr>
<tr>
<td>D</td>
<td>$38118$</td>
</tr>
</tbody>
</table>

$\Delta H_f/(kJ mol^{-1}) = 163.2 - 33331 = 57.15$
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: C_{10}H_{14}, C_6H_2(CH_3)_4
Molecular Weight: 134.218
Melting Point (°C):
-24.1 (Stephenson & Malanowski 1987)
Boiling Point (°C):
198 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
0.8903 (Weast 1982–83)
Molar Volume (cm³/mol):
150.8 (20°C, calculated-density)
184.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{fus} (kJ/mol):
12.93 (Chickos et al. 1999)
Entropy of Fusion ΔS_{fus} (J/mol K):
52.01, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°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°C, summary of literature data, temp range 40.6–197.9°C, Stull 1947)
67.10 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.0769 − 1674.00/(200.94 + t°C); temp range 95–240°C (Antoine eq. for liquid state, Dreisbach 1955)
62.22* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.70779 − 1675.43/(201.14 + t°C); temp range 74.5–228.3°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = [−0.2185 × 12358.4/(T/K)] + 8.680246; temp range 40.6–197.9°C (Antoine eq., West 1972–73)
log (P/atm) = (1 − 471.208/T) × 10^4(0.891876 − 6.64575 × 10^3+ 5.21861 × 10^3·T); 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 (P/mmHg) = 7.0779 − 1675.43/(201.14 + t°C); temp range 75–228°C (Antoine eq., Dean 1985, 1992)
62.23 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.2028 − 1675.43/(−72.01 + T/K); temp range 348–502 K (Antoine eq., Stephenson & Malanowski 1987)
log (P/mmHg) = −3.9778 − 2.960 × 10^3/(T/K) + 7.3226-log (T/K) − 1.7725 × 10^2·(T/K) + 8.6365 × 10^6·(T/K)^2, temp range 249–679 K (Yaws 1994)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
4.04 (generator column-HPLC/UV, Wasik et al. 1982)
4.17 (HPLC-k’ correlation, Hammers et al. 1982)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

#### Half-Lives in the Environment:

**TABLE 3.1.121.1**

Reported vapor pressures of 1,2,3,5-tetramethylbenzene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$P/Pa$</th>
<th>$t/°C$</th>
<th>$P/Pa$</th>
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<tbody>
<tr>
<td>40.6</td>
<td>133.3</td>
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<td>65.8</td>
<td>666.6</td>
<td>88.9</td>
<td>2666</td>
</tr>
<tr>
<td>77.8</td>
<td>1333</td>
<td>98</td>
<td>4000</td>
</tr>
<tr>
<td>91</td>
<td>2666</td>
<td>104.8</td>
<td>5333</td>
</tr>
<tr>
<td>105.8</td>
<td>5333</td>
<td>110.3</td>
<td>6666</td>
</tr>
<tr>
<td>115.4</td>
<td>7999</td>
<td>115</td>
<td>7999</td>
</tr>
<tr>
<td>128.3</td>
<td>13332</td>
<td>122.6</td>
<td>10666</td>
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<tr>
<td>149.9</td>
<td>26664</td>
<td>128.8</td>
<td>13332</td>
</tr>
<tr>
<td>173.7</td>
<td>53329</td>
<td>140.7</td>
<td>19998</td>
</tr>
<tr>
<td>197.9</td>
<td>101325</td>
<td>149.6</td>
<td>26664</td>
</tr>
<tr>
<td>mp/°C</td>
<td>–24.0</td>
<td>156.9</td>
<td>33331</td>
</tr>
<tr>
<td></td>
<td></td>
<td>163</td>
<td>39997</td>
</tr>
<tr>
<td></td>
<td></td>
<td>173.2</td>
<td>53329</td>
</tr>
<tr>
<td></td>
<td></td>
<td>181.5</td>
<td>66661</td>
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<tr>
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<td></td>
<td>188.5</td>
<td>79993</td>
</tr>
</tbody>
</table>

**Stull 1947**

**Zwolinski & Wilhoit 1971**

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$P/mmHg$</th>
<th>$A$</th>
<th>$B$</th>
<th>$C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>74.5</td>
<td>1333</td>
<td>94.68</td>
<td>93326</td>
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<tr>
<td>88.9</td>
<td>2666</td>
<td>195.83</td>
<td>95992</td>
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<td>98</td>
<td>4000</td>
<td>196.95</td>
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<td>104.8</td>
<td>5333</td>
<td>198.05</td>
<td>101325</td>
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<tr>
<td>110.3</td>
<td>6666</td>
<td>198.05</td>
<td>101325</td>
<td></td>
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<tr>
<td>115</td>
<td>7999</td>
<td>eq. 2</td>
<td>P/mmHg</td>
<td></td>
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<tr>
<td>122.6</td>
<td>10666</td>
<td>A</td>
<td>7.0779</td>
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<td>128.8</td>
<td>13332</td>
<td>B</td>
<td>1675.43</td>
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<tr>
<td>140.7</td>
<td>19998</td>
<td>C</td>
<td>201.14</td>
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<td>149.6</td>
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<td>156.9</td>
<td>33331</td>
<td>bp/°C</td>
<td>198.05</td>
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<tr>
<td>163</td>
<td>39997</td>
<td>$\Delta H_f/(kJ mol^{-1}) = \Delta H_f$</td>
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<tr>
<td>173.2</td>
<td>53329</td>
<td>at 25°C</td>
<td>55.82</td>
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<tr>
<td>181.5</td>
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<td>at bp</td>
<td>43.81</td>
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<td></td>
</tr>
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</table>

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**FIGURE 3.1.1.21.1** Logarithm of vapor pressure versus reciprocal temperature for 1,2,3,5-tetramethylbenzene.
3.1.1.22 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: C_{10}H_{14}, C_6H_2(CH_3)_4
Molecular Weight: 134.218

Melting Point (°C):
79.3 (Lide 2003)

Boiling Point (°C):
196.8 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm³ at 20°C): 0.838

Molar Volume (cm³/mol):
160.1 (20°C, calculated-density)
184.8 (calculated-Le Bes method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):
21.0 (Dreisbach 1955; Tsonopoulos & Prausnitz 1971)
20.88 (Chickos et al. 1999)

Entropy of Fusion ΔS_{fus} (J/mol K):
59.83 (Tsonopoulos & Prausnitz 1971)
59.25, 46.7 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.293 (mp at 79.3°C)

Water Solubility (g/m³ or mg/L at 25°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 γ_W, Hafkenscheid & Tomlinson 1983)
17.2, 18.6, 28.2 (15, 25, 35°C, RP-HPLC-k′ correlation, Finizio & Di Guardo 2001)

Vapor Pressure (Pa at 25°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* (1.75°C, mercury manometer, measured range –1.7–1.75 °C, Linder 1931)
133.3* (45°C, summary of literature data, temp range 45–195.9°C, Stull 1947)
70.9 (extrapolated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 7.0790 – 1671.0/(201.23 + t/°C); temp range 95–240°C (Antoine eq., Chao et al. 1983)
65.9 (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = 7.0800 – 1672.43/(201.43 + t/°C); temp range 73.6–227°C (Antoine eq., Zwolinski & Wilhoit 1971)

log (P/mmHg) = [–0.2185 × 12582.6/(T/K)] + 8.822113; temp range 45–195.9°C (Antoine eq., Weast 1972–73)
65.9 (extrapolated-Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.0800 – 1672.43/(201.43 + t/°C); temp range 74–277°C (Antoine eq., Dean 1985, 1992)
65.9 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P_kPa) = 6.2049 – 1672.43/(–71.72 + T/K); temp range 353–500 K (Antoine eq., Stephenson & Malanowski 1987)
\[
\log(P/\text{mmHg}) = -51.3593 - 1.6523 \times 10^3/(T/\text{K}) + 26.656 \log(T/\text{K}) - 3.5721 \times 10^{-2}(T/\text{K}) + 1.5018 \times 10^{-5}(T/\text{K})^2,
\]

temp range 352–Y675K (Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):
2541 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):
4.00 (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, \( \log K_{\text{oa}} \):

Bioconcentration Factor, \( \log B_{\text{CF}} \):

Sorption Partition Coefficient, \( \log K_{\text{oc}} \):
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 \( f_{\text{oc}} \) of 0.006 and measured \( K_p = 3.42 \text{ mL/g.} \), Abdul et al. 1990)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):
Volatilization:
Photolysis:
Oxidation: rate constant \( k = 1.1 \times 10^4 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} \) 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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\log P &= A - B/(C + t/^\circ C) \\
\log P &= A - B/(T/K) - C\cdot\log(T/K)
\end{align*}
\]

Linder 1931  Stull 1947  Zwolinski & Wilhoit 1971

<table>
<thead>
<tr>
<th>Hg manometer</th>
<th>summary of literature data</th>
<th>selected values</th>
</tr>
</thead>
<tbody>
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<td>t/^\circ C</td>
<td>P/Pa</td>
<td>t/^\circ C</td>
</tr>
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<td>–1.7</td>
<td>1.733</td>
<td>45</td>
</tr>
<tr>
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<td>21.33</td>
<td>63</td>
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<td>1.3</td>
<td>4.4</td>
<td>74.6</td>
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<td>1.75</td>
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</tr>
<tr>
<td>mp/^\circ C</td>
<td>79.5</td>
<td></td>
</tr>
</tbody>
</table>

Experimental data

\[\Delta H_f/(kJ \text{ mol}^{-1}) = 75\]

**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: C_{11}H_{16}, C_6H(CH_3)_5
Molecular Weight: 148.245
Melting Point (°C):
54.5 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
232 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C):
0.917, 0.913 (20°C, 25°C, Dreisbach 1955)
0.917 (Weast 1982–83)
Molar Volume (cm³/mol):
161.7 (20°C, calculated from density)
207.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion ΔH_{ fus} (kJ/mol):
12.34 (Tsonopoulos & Prausnitz 1971)
1.98, 10.67; 12.65 (23.65, 55.05°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion ΔS_{ fus} (J/mol K):
37.70 (Tsonopoulos & Prausnitz 1971)
39.33, 47.3 (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K.), F: 0.514 (mp at 54.5°C)
Water Solubility (g/m³ or mg/L at 25°C):
15.6 (Deno & Berkheimer 1960)
15.52 (calculated-K_{ OW}, Yalkowsky et al. 1983)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
13.84 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.13756 – 1833.8/(199.0 + t°C); temp range 125–280°C (Antoine eq. for liquid state, Dreisbach 1955)
9.52 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_l/kPa) = 6.3509 – 1867/(–75.15 + T/K); temp range 338–503 K (Antoine eq., Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ 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 $K_{OA}$:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:
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: C₁₁H₁₆, C₆H₅(CH₂)₄CH₃  
Molecular Weight: 148.245

Melting Point (°C):  
−75 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Boiling Point (°C):  
205.4 (Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):  
0.8585 (Weast 1982–83)

Molar Volume (cm³/mol):  
172.7 (20°C, calculated from density)  
207.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion $\Delta H_{fus}$ (kJ/mol):

Entropy of Fusion $\Delta S_{fus}$ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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°C, Owens et al. 1986)  
$\ln x = –387.920 + 16274.64/(T/K) + 55.9266·\ln (T/K)$; temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)

Vapor Pressure (Pa at 25°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)  
$\log (P/mmHg) = 7.04709 – 1670.68/(195.6 + t/°C)$; temp range 105–270°C (Antoine eq. for liquid state, Dreisbach 1955)  
43.7* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)  
$\log (P/mmHg) = 6.97833 – 1639.91/(194.76 + t/°C)$; temp range 80–237°C (Antoine eq., Zwolinski & Wilhoit 1971)  
$\log (P/mmHg) = 34.2755 – 3.6829 \times 10^{-3}/(T/K) – 9.3387·\log (T/K) + 2.7727 \times 10^{-3}/(T/K) – 8.8315 \times 10^{-15}/(T/K)^2$, temp range 198–680 K (Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):  
600 (calculated-P/C, Mackay & Shiu 1981)  
617 (calculated-C_a/C_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 $K_{ow}$:  
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 $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environment Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k = 5.0 \times 10^4$ cm$^3$ mol$^{-1}$ s$^{-1}$ for the reaction with ozone at 300 K (Lyman 1982).
- Hydrolysis:
- Biodegradation:
- Bioconcentration:

Half-Lives in the Environment:

<table>
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<tr>
<th>t/°C</th>
<th>S/g·m$^{-3}$</th>
<th>7</th>
<th>3.48</th>
<th>80</th>
<th>1333</th>
<th>283.18</th>
<th>95992</th>
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<tbody>
<tr>
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<td>94</td>
<td>2666</td>
<td>203.16</td>
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<td></td>
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</tr>
<tr>
<td>12.5</td>
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<td>103.3</td>
<td>4000</td>
<td>204.33</td>
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<td>205.46</td>
<td>101325</td>
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</tr>
<tr>
<td>20</td>
<td>3.18</td>
<td>120.6</td>
<td>7999</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>3.37</td>
<td>128.36</td>
<td>10666</td>
<td>log $P = A - B/(C + t/°C)$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>3.61</td>
<td>134.65</td>
<td>13332</td>
<td>Antoine eq. $P/mmHg$</td>
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<tr>
<td>35</td>
<td>3.92</td>
<td>146.73</td>
<td>19998</td>
<td>A</td>
<td>6.97833</td>
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<td></td>
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<tr>
<td>40</td>
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<td>155.85</td>
<td>26664</td>
<td>B</td>
<td>1639.91</td>
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<tr>
<td>45</td>
<td>4.69</td>
<td>163.27</td>
<td>33331</td>
<td>C</td>
<td>194.76</td>
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</tr>
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</table>

$\Delta H_{\text{sol}}/(kJ mol^{-1}) = 6.50$ at 25°C

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>179.97</th>
<th>53329</th>
<th>bp/°C</th>
<th>205.46</th>
</tr>
</thead>
<tbody>
<tr>
<td>188.45</td>
<td>66661</td>
<td>$\Delta H_{\text{v}}/(kJ mol^{-1})$</td>
<td>196.68</td>
<td>79993</td>
<td>55.06</td>
</tr>
<tr>
<td>202</td>
<td>93326</td>
<td>at 25°C</td>
<td>202.59</td>
<td>94659</td>
<td>41.21</td>
</tr>
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</table>
FIGURE 3.1.1.24.1 Logarithm of mole fraction solubility (ln 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

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Common Name:</strong></td>
<td>n-Hexamethylbenzene</td>
</tr>
<tr>
<td><strong>Synonym:</strong></td>
<td>mellitene</td>
</tr>
<tr>
<td><strong>Chemical Name:</strong></td>
<td>n-hexamethylbenzene</td>
</tr>
<tr>
<td><strong>CAS Registry No:</strong></td>
<td>87-95-4</td>
</tr>
<tr>
<td><strong>Molecular Formula:</strong></td>
<td>C₁₂H₁₈, C₆(CH₃)₆</td>
</tr>
<tr>
<td><strong>Molecular Weight:</strong></td>
<td>162.271</td>
</tr>
<tr>
<td><strong>Melting Point (°C):</strong></td>
<td>165.5 (Lide 2003)</td>
</tr>
<tr>
<td><strong>Boiling Point (°C):</strong></td>
<td>263.4 (Weast 1982–83)</td>
</tr>
<tr>
<td><strong>Density (g/cm³ at 25°C):</strong></td>
<td>1.063 (Weast 1982–83)</td>
</tr>
<tr>
<td><strong>Molar Volume (cm³/mol):</strong></td>
<td>152.6 (25°C, calculated-density)</td>
</tr>
<tr>
<td><strong>Enthalpy of Fusion ΔHₚₜₜ (kJ/mol):</strong></td>
<td>20.46 (Tsonopoulos &amp; Prausnitz 1971)</td>
</tr>
<tr>
<td><strong>Entropy of Fusion ΔSₚₜₜ (J/mol K):</strong></td>
<td>46.44 (Tsonopoulos &amp; Prausnitz 1971)</td>
</tr>
<tr>
<td><strong>Water Solubility (g/m³ or mg/L at 25°C):</strong></td>
<td>0.235 (generator column-GC, Doucette &amp; Andren 1988)</td>
</tr>
<tr>
<td><strong>Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):</strong></td>
<td>1.004* (41.0°C, transpiration method, measured range 41–90.5°C, Overberger et al. 1969)</td>
</tr>
<tr>
<td><strong>Henry’s Law Constant (Pa m³/mol):</strong></td>
<td>4.61 (generator column-HPLC, Wasik et al. 1982)</td>
</tr>
</tbody>
</table>


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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 K_{OA}:
6.31 (calculated-S_{oc} and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

Volatileization:

Photolysis:

Oxidation: rate constant k = 2.4 × 10^5 cm^3 mol^-1 s^-1 for the reaction with ozone at 300K (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

<table>
<thead>
<tr>
<th>Overberger et al. 1969</th>
<th>Ambrose et al. 1976</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>transpiration method</strong></td>
<td><strong>diaphragm gauge</strong></td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>41.07</td>
<td>1.004</td>
</tr>
<tr>
<td>49.11</td>
<td>2.306</td>
</tr>
<tr>
<td>54.68</td>
<td>3.912</td>
</tr>
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<td>62.62</td>
<td>8.015</td>
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<td>68.71</td>
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<td>68.72</td>
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<tr>
<td>84.2</td>
<td>48.3</td>
</tr>
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<td>89.46</td>
<td>72</td>
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<tr>
<td>89.48</td>
<td>72.16</td>
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<td>90.54</td>
<td>77.91</td>
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<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>
FIGURE 3.1.25.1 Logarithm of vapor pressure versus reciprocal temperature for \( n \)-hexamethylbenzene.
3.1.1.26  \( n \)-Hexylbenzene

![Chemical Structure of \( n \)-Hexylbenzene](image)

**Common Name:** \( n \)-Hexylbenzene  
**Synonym:** 1-phenylhexane, hexylbenzene  
**Chemical Name:** \( n \)-hexylbenzene  
**CAS Registry No:** 1077-16-3  
**Molecular Formula:** \( C_{12}H_{18} \), \( C_6H_5(CH_2)_5CH_3 \)  
**Molecular Weight:** 162.271  
**Melting Point (°C):**  
\(-61.0\) (Dreisbach 1955; Lide 2003)  
**Boiling Point (°C):**  
226.1 (Lide 2003)  
**Density (g/cm\(^3\) at 20°C):**  
0.8613 (Weast 1982–83)  
**Molar Volume (cm\(^3\)/mol):**  
188.4 (20°C, calculated from density)  
229.2 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):**  
**Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):**  
**Fugacity Ratio at 25°C, \( F \):** 1.0  
**Water Solubility (g/m\(^3\) or mg/L at 25°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  
0.995*  
0.902*  
\[ \ln x = -429.463 + 18024.83/(T/K) + 61.9402 \cdot \ln (T/K); \text{ temp range 290–400 K (eq. derived from literature calorimetric and solubility data, Tsonopoulos 1999)} \]  
**Vapor Pressure (Pa at 25°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  
13.61*  
\[ \log (P/\text{mmHg}) = 7.18284 - 1813.74/(195.5 + t/°C); \text{ temp range 120–290°C (Antoine eq. for liquid state, Dreisbach 1955)} \]  
\[ \log (P/\text{mmHg}) = 6.9853 - 1700.5/(188.2 + t/°C); \text{ temp range 96–258°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]  
\[ \log (P/\text{mmHg}) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K)^2; \text{ temp range 212–698 K (Yaws 1994)} \]  
10.52*  
\[ \log (P/\text{mmHg}) = 7.18284 - 1813.74/(195.5 + t/°C); \text{ temp range 263.88–462.97 K (Kasehgari et al. 1993)} \]  
\[ \log (P/\text{mmHg}) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K)^2; \text{ temp range 212–698 K (Yaws 1994)} \]  
**Henry’s Law Constant (Pa m\(^3\)/mol):**  
1977  
2172  
\[ \log (P/\text{mmHg}) = 7.18284 - 1813.74/(195.5 + t/°C); \text{ temp range 263.88–462.97 K (Kasehgari et al. 1993)} \]  
\[ \log (P/\text{mmHg}) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K)^2; \text{ temp range 212–698 K (Yaws 1994)} \]  
**Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):**  
5.25  
5.52  
5.24  
\[ \log (P/\text{mmHg}) = 7.18284 - 1813.74/(195.5 + t/°C); \text{ temp range 263.88–462.97 K (Kasehgari et al. 1993)} \]  
\[ \log (P/\text{mmHg}) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K)^2; \text{ temp range 212–698 K (Yaws 1994)} \]  
\[ \log (P/\text{mmHg}) = 6.7694 - 3.6050 \times 10^3/(T/K) + 3.3416 \cdot \log (T/K) - 1.5306 \times 10^{-2} \cdot (T/K)^2; \text{ temp range 212–698 K (Yaws 1994)} \]
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 K_{OC}:

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 3.1.1.26.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported aqueous solubilities of ( n )-hexylbenzene at various temperatures</td>
</tr>
<tr>
<td>( t/°C )</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>8</td>
</tr>
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<td>9</td>
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<td>11</td>
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<td>12</td>
</tr>
<tr>
<td>13</td>
</tr>
<tr>
<td>14</td>
</tr>
<tr>
<td>15</td>
</tr>
<tr>
<td>16.01</td>
</tr>
</tbody>
</table>
| 17 | 0.919 | 18 | 0.91 | \( \Delta H_{\text{sol}}/(kJ \cdot mol^{-1}) = 7.60 \) at \( 25°C \)
| 19 | 0.921 | \( \Delta H_{\text{sol}}/(kJ \cdot mol^{-1}) = 8.0 \) at \( 25°C \)

*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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>selected values</th>
<th>Kasehgari et al. 1993</th>
<th>static method</th>
<th>Mokbel et al. 1998</th>
<th>static method</th>
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</thead>
<tbody>
<tr>
<td>(t/°C)</td>
<td>(P/Pa)</td>
<td>(T/K)</td>
<td>(P/Pa)</td>
<td>(T/K)</td>
</tr>
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<td>1333</td>
<td>273.73</td>
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<td>111</td>
<td>2666</td>
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<td>293.66</td>
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<td>138.4</td>
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<td>422.76</td>
<td>11828</td>
<td>412.76</td>
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<td>432.75</td>
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<td>226.1</td>
<td>101325</td>
<td>eq. 2</td>
<td>P/kPa</td>
<td>data fitted to Wagner eq.</td>
</tr>
<tr>
<td>Antoine eq.</td>
<td>P/mmHg</td>
<td>A 6.9853</td>
<td>B 1946.435</td>
<td>C 208.935</td>
</tr>
<tr>
<td>A</td>
<td>6.9853</td>
<td>B 1700.5</td>
<td>C 1882.2</td>
<td></td>
</tr>
<tr>
<td>bp/°C</td>
<td>226.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\Delta H_v/(kJ \text{ mol}^{-1})) at 25°C</td>
<td>60</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>at bp</td>
<td>43.1</td>
<td></td>
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</tr>
</tbody>
</table>
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: \( C_{13}H_{20}, C_6H_5(CH_2)_6CH_3 \)
Molecular Weight: 176.298
Melting Point (°C):
\(-48\)  
(Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
240  
(Lide 2003)
Density (g/cm³):
0.8567  
(20°C, Weast 1982–83)
Molar Volume (cm³/mol):
205.8  
(20°C, calculated-density)
251.4  
(calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol): 
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
0.686; 0.925  
(calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
133.3* (66.2°C, summary of literature data, temp range 66.2–233°C, Stull 1947)
1333* (112°C, derived from compiled data, temp range 112–279°C (Antoine eq., Zwolinski & Wilhoit 1971)
\[ \log (P/\text{mmHg}) = 7.0006 - 1761.2/(181.5 + t/°C) \]; temp range 112–279°C (Antoine eq., Zwolinski & Wilhoit 1971)
\[ \log (P/\text{kPa}) = 6.1255 - [1761.2/(T - 91.65)]; \text{temp range 423–527 K (liquid, Antoine equation, Stephenson & Malanowski 1987)} \]
\[ \log (P/\text{mmHg}) = 89.2811 - 6.4093 \times 10^3/(T/K) - 29.248 \log (T/K) + 1.0328 \times 10^{-2} \times (T/K) + 6.2451 \times 10^{-14} \times (T/K)^2, \]  
temp range 225–714 K (Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \( K_{\text{ow}} \):
5.768  
(HPLC-k’ correlation, Hanai & Hubert 1981)
5.37  
(HPLC-k’ correlation, Ritter et al. 1995)
Octanol/Air Partition Coefficient, log \( K_{\text{oa}} \):
Bioconcentration Factor, log BCF or log \( K_{\text{bi}} \):
Sorption Partition Coefficient, log \( K_{\text{oc}} \):
Environmental Fate Rate Constants, k, and Half-Lives, \( t_{1/2} \):
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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\log P &= A - \frac{B}{T/K} - C \log (T/K) \quad (4)
\end{align*}
\]

Stull 1947

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Zwolinski & Wilhoit 1971

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Summary of literature data

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FIGURE 3.1.1.27.1 Logarithm of vapor pressure versus reciprocal temperature for heptylbenzene.
3.1.1.28  \textit{n}-Octylbenzene

Common Name: \textit{n}-Octylbenzene  
Synonym: 1-phenyloctane, octylbenzene  
Chemical Name: \textit{n}-octylbenzene  
CAS Registry No: 2189-60-8  
Molecular Formula: C\textsubscript{14}H\textsubscript{22}, C\textsubscript{6}H\textsubscript{5}(CH\textsubscript{2})\textsubscript{7}CH\textsubscript{3}  
Molecular Weight: 190.325  
Melting Point (°C): -36  (Lide 2003)  
Boiling Point (°C): 264  (Lide 2003)  
Density (g/cm\textsuperscript{3}): 0.8582  (20°C, Weast 1982–83)  
Molar Volume (cm\textsuperscript{3}/mol): 222.2  (20°C, calculated-density)  
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol): 29.96  (Chickos et al. 1999)  
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K): 127.91, 110.4  (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)  
Fugacity Ratio at 25°C, F: 1.0  
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C): 0.219; 0.204  (calculated-regression eq.; calculated-molar volume correlation, Wang et al. 1992)  
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section): 1333*  (127°C, derived from compiled data, temp range 127–264.4°C, Zwolinski & Wilhoit 1971)  
log (P/mmHg) = 7.0086 – 1812.2/(174.6 + t/°C); temp range 127–298°C  
log (P/kPa) = 8.35571 – 3293.744/(T/K); temp range 368–400 K  
log (P/mmHg) = 1.8919 – 4.1324 × 10\textsuperscript{3}/(T/K) + 6.1473·log (T/K) – 2.0294 × 10\textsuperscript{-2}·(T/K)\textsuperscript{2}, temp range 237–729 K  
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C): 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 K\textsubscript{OA}:
Bioconcentration Factor, log BCF or log $K_B$;

Sorption Partition Coefficient, log $K_{OC}$;

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

\[
\log P = A - B/(T/K) \quad (1)
\]

\[
\ln P = A - B/(T/K) \quad (1a)
\]

\[
\log P = A - B/(C + t/°C) \quad (2)
\]

\[
\ln P = A - B/(C + t/°C) \quad (2a)
\]

\[
\log P = A - B/(C + T/K) \quad (3)
\]

\[
\log P = A - B/(T/K) - C\cdot\log (T/K) \quad (4)
\]

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**Antoine eq.:**

- $A = \text{7.0086}$
- $B = \text{1812.2}$
- $C = \text{174.6}$
- $\text{bp} = \text{264.4}$

$\Delta H_v/(\text{kJ mol}^{-1}) =$

- at $25^\circ\text{C}$: $\text{69.96}$
- at $\text{bp}$: $\text{46.9}$
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: \( C_{15}H_{24}, C_6H_5(CH_2)_8CH_3 \)
Molecular Weight: 204.352

Melting Point (°C):
-24 (Dreisbach 1955; Lide 2003)

Boiling Point (°C):
280.5 (Lide 2003)

Density (g/cm³):
- 0.8558, 0.8522 (20°C, 25°C, Dreisbach 1955)
- 0.8584 (20°C, Weast 1982–83)

Molar Volume (cm³/mol):
- 238.1 (20°C, calculated-density)
- 295.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C, \( F \): 1.0

Water Solubility (g/m³ or mg/L at 25°C):
- 0.0725; 0.112 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)

Vapor Pressure (Pa at 25°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)
- \( \log (P/\text{mmHg}) = 7.19041 – 1991.0/(180.0 + t/°C); \) temp range 165–330°C (Antoine eq. for liquid state, Dreisbach 1955)
- 1333* (142°C, derived from compiled data, temp range 142–282°C, Zwolinski & Wilhoit 1971)
- \( \log (P/\text{mmHg}) = 7.0245 – 1862.6/(167.5 + t/°C); \) temp range 142–316°C (Antoine eq., Zwolinski & Wilhoit 1971)
- 2.906* (43°C, gas saturation, measured range 43–142°C, Allemand et al. 1986)
- 0.338 (GC-RT correlation, Sherblom et al. 1992)
- \( \log (P/\text{mmHg}) = -0.9235 – 4.2232 \times 10^3/(T/K) + 7.3073 \times 10^2/(T/K) – 2.0964 \times 10^3/(T/K)^2 + 9.7152 \times 10^4/(T/K)^3, \) temp range 249–741 K (Yaws 1994)
- 0.8747* (30.52°C, static method, measured range 313.67–466.46 K, Mokbel et al. 1998)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
- 6.828 (HPLC-k’ correlation, Hanai & Hubert 1981)
- 6.63, 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, \( \log K_{\text{OA}} \):

Bioconcentration Factor, \( \log BCF \) or \( \log K_{\text{B}} \):

Sorption Partition Coefficient, \( \log K_{\text{OC}} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\cdot\log (T/K) \quad (4)
\end{align*}
\]

Zwolinski & Wilhoit 1971

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Allemand et al. 1986

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Mokbel et al. 1998

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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: \( \text{C}_{16}\text{H}_{26}, \text{C}_6\text{H}_5(\text{CH}_2)_9\text{CH}_3 \)  
Molecular Weight: 218.337

Melting Point (°C):  
-14.4 (Dreisbach 1955, Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):  
293 (Lide 2003)

Density (g/cm\(^3\)):  
0.85553, 0.85189 (20°C, 25°C, Camin et al. 1954; Dreisbach 1955)

Molar Volume (cm\(^3\)/mol):  
255.3 (20°C, calculated-density)  
318.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):  

Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):  

Fugacity Ratio at 25°C, \( F \): 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°C):  
2.50 (vapor-phase saturation, shake flask-GC, Sherblom et al. 1992)  
5.59, 8.47, 10.55 (calculated-\( V_M \), \( K_{\text{ow}} \), 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°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):  
\[
\log (P/\text{mmHg}) = 7.03642 - 1904.132/(160.318 + t/°C); \text{temp range 202.9–297.9°C (Antoine eq., manometer measurements, Camin et al. 1954)}
\]  
0.20 (extrapolated-Antoine eq., Dreisbach 1961)  
\[
\log (P/\text{mmHg}) = 7.27177 - 2107.7/(180.0 + t/°C); \text{temp range 185–345°C (Antoine eq. for liquid state, Dreisbach 1955)}
\]  
1333* (155.1°C, derived from compiled data, temp range 155.1–297.89°C, Zwolinski & Wilhoit 1971)  
\[
\log (P/\text{mmHg}) = 7.03642 - 1904.132/(160.318 + t/°C); \text{temp range 155.1–322.9°C (Antoine eq., Zwolinski & Wilhoit 1971)}
\]  
\[
\log (P/\text{kPa}) = 6.16274 - 1905.56/(160.503 + t/°C); \text{temp range 203–297.8°C (Antoine eq. from reported exp. data of Camin et al. 1954, Boublík et al. 1984)}
\]  
\[
\log (P/\text{kPa}) = 4.03653 - 876.208/(T/K – 203.15); \text{temp range 317–427 K (liquid, Antoine equation, Stephenson & Malanowski 1987)}
\]  
\[
\log (P/\text{kPa}) = 6.15658 - [1900.916/(T/K – 113.16)]; \text{temp range 475–571 K (liquid, Antoine equation, Stephenson & Malanowski 1987)}
\]  
0.133, 0.127 (P\(_{L}\), GC-RT correlation, Sherblom et al. 1992)  
0.707* (39.85°C, static method, measured range 313.0–433.23 K, Kasehgari et al. 1993)  
\[
\log (P/\text{kPa}) = 6.37655 - 2098.329/(180.620 + t/°C); \text{temp range 313.0–433.23 K (static method, Kasehgari et al. 1993)}
\]  
\[
\log (P/\text{mmHg}) = -4.4754 - 4.4669 \times 10^5/(T/K) + 9.1965 \log (T/K) - 2.4010 \times 10^{-2}(T/K) + 1.0848 \times 10^{-5}(T/K)^2; \text{temp range 259–753 K (Yaws 1994)}
\]
Henry's Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 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, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \) or \( \log K_B \):

Sorption Partition Coefficient, \( \log K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 3.1.1.30.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of decylbenzene at various temperatures and the coefficients for the vapor pressure equations</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\text{log } P &= A - B/(T/K) \quad (1) \\
\text{ln } P &= A - B/(T/K) \quad (1a) \\
\text{log } P &= A - B/(C + t/°C) \quad (2) \\
\text{ln } P &= A - B/(C + t/°C) \quad (2a) \\
\text{log } P &= A - B/(C + T/K) \quad (3) \\
\text{log } P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]


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<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>T/K</th>
<th>P/Pa</th>
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<td>1333</td>
<td>eq. 2</td>
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<td>217.156</td>
<td>13088</td>
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<td>B</td>
<td>1904.132</td>
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<td>230.476</td>
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<td>5333</td>
<td>C</td>
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<td>278.950</td>
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<td>( \Delta H_v/(kJ \text{ mol}^{-1}) = )</td>
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<td>296.370</td>
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<td>297.89</td>
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</table>

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FIGURE 3.1.130.1 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: \( \text{C}_{17}\text{H}_{28}, \text{C}_{6}\text{H}_{5}(\text{CH}_{2})_{10}\text{CH}_{3} \)
Molecular Weight: 232.404
Melting Point (°C):
\(-5.0\) (Dreisbach 1955; Lide 2003)
Boiling Point (°C):
316 (Dreisbach 1955; Lide 2003)
Density (g/cm\(^3\)):
0.8553, 0.8517 (20°C, 25°C, Dreisbach 1961)
Molar Volume (cm\(^3\)/mol):
271.7 (20°C, calculated-density)
340.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\(^3\) or mg/L at 25°C):
0.00702; 0.00377 (calculated-regression eq., calculated-molar volume correlation, Wang et al. 1992)
Vapor Pressure (Pa at 25°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 (P/mmHg) = 7.34672 − 2215.1/(180.0 + t°C); temp range 195–375°C (Antoine eq. for liquid state, Dreisbach 1955)
1333* (168°C, derived from compiled data, temp range 168–313.2°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.0509 − 1944.1/(153.0 + t°C); temp range 168–349°C (Antoine eq., Zwolinski & Wilhoit 1971)
0.050, 0.047 (\( P_{L} \); GC-RT correlation, Sherblom et al. 1992)
log (P/mmHg) = 124.1549 − 8.8970 × 10\(^{3}\)/(T/K) − 41.223 log (T/K) + 1.3662 × 10\(^{-3}\)(T/K)\(^2\); temp range 268–764 K (Yaws 1994)
0.7156* (50.42°C, static method, measured range 323.57–467.33°C, data fitted to Wagner eq., Mokbel et al. 1998)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
Octanol/Air Partition Coefficient, \( \log K_{\text{OA}} \):
Bioconcentration Factor, \( \log BCF \) or \( \log K_{\text{B}} \):
Sorption Partition Coefficient, \( \log K_{\text{OC}} \):
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{1/2} \):
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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\log P &= A - \frac{B}{T/K + t/°C} \quad (2) \\
\log P &= A - \frac{B}{T/K} - C \log (T/K) \\
\log P &= A - \frac{B}{C + t/°C} \\
\log P &= A - \frac{B}{T/K} (3)
\end{align*}
\]

Zwolinski & Wilhoit 1971

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<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<td>309.2</td>
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<td>185</td>
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<td>196</td>
<td>4000</td>
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<td>98659</td>
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<td>204</td>
<td>5333</td>
<td>313.2</td>
<td>101325</td>
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<td>210.3</td>
<td>6666</td>
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<tr>
<td>215.7</td>
<td>7999</td>
<td>eq. 2</td>
<td>P/mmHg</td>
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<td>224.7</td>
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<td>ΔHv/(kJ mol⁻¹)</td>
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<td>284</td>
<td>53329</td>
<td>at 25°C</td>
<td>422.19</td>
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Mokbel et al. 1998

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**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: \( \text{C}_{18}\text{H}_{30}, \text{C}_{6}\text{H}_{5}(\text{CH}_{2})_{11}\text{CH}_{3} \)
Molecular Weight: 246.431
Melting Point (°C): 3.0 (Dreisbach 1955; Lide 2003)
Boiling Point (°C): 328 (Lide 2003)
Density (g/cm³): 0.8551, 0.8516 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol): 288.2 (20°C, calculated-density)
362.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C, \( F \): 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
26.66* (78.4°C, ebulliometry-McLeod gauge, measured range 78.4–288.6°C, Myers & Fenske 1955)
0.032 (extrapolated-Antoine eq., Dreisbach 1955)
log (P/mmHg) = 7.41934 – 2319.2/(180.0 + t/°C); temp range 210–385°C (Antoine eq. for liquid state, Dreisbach 1955)
1333* (181°C, derived from compiled data, temp range 181–327.6°C, Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.0693 – 1981.6/(145.5 + t/°C); temp range 181–363°C (Antoine eq., Zwolinski & Wilhoit 1971)
1.08* (53.7°C, gas saturation, measured range 53.7–192.7°C, Allemand et al. 1986)
0.019, 0.017 (P L, GC-RT correlation, Sherblom et al. 1992)
0.727* (69.771°C, static method, measured range 332.92–453.26 K, Kasehgari et al. 1993)
log (P/kPa) = 6.66087 – 2371.902/(182.311 + t/K); temp range 276–774 K (Yaws 1994)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
8.65 (RP-HPLC-k′ correlation, Sherblom et al. 1992)
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
Bioconcentration Factor, log BCF or log \( K_{\text{B}} \):
Sorption Partition Coefficient, log \( K_{\text{OC}} \):
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{\frac{1}{2}} \):
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

\[
\log P = A - B/(T/K) \quad (1) \\
\ln P = A - B/(T/K) \quad (1a) \\
\log P = A - B/(C + t/°C) \quad (2) \\
\ln P = A - B/(C + t/°C) \quad (2a) \\
\log P = A - B/(C + T/K) \quad (3) \\
\log P = A - B/(T/K) - C\log (T/K) \quad (4)
\]

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<td><strong>static method</strong></td>
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</tr>
<tr>
<td>225.4</td>
<td>19998</td>
<td>327.6</td>
<td>101325</td>
</tr>
<tr>
<td>235.8</td>
<td>26664</td>
<td>329.5</td>
<td>103992</td>
</tr>
<tr>
<td>250.3</td>
<td>39997</td>
<td>332.6</td>
<td>106661</td>
</tr>
<tr>
<td>262.0</td>
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<td>335.3</td>
<td>109326</td>
</tr>
<tr>
<td>270.4</td>
<td>66661</td>
<td>338.0</td>
<td>112092</td>
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<td>340.7</td>
<td>114858</td>
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<td>93326</td>
<td>343.4</td>
<td>117624</td>
</tr>
<tr>
<td>288.6</td>
<td>101325</td>
<td>bp/°C</td>
<td>327.6</td>
</tr>
</tbody>
</table>

\[ \Delta H_v/(kJ \cdot mol^{-1}) \]

at 25°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: \(C_{19}H_{32}, C_6H_5(CH_2)_{12}CH_3\)
Molecular Weight: 260.457

Density (g/cm³):
- 0.8550, 0.8515 (20°C, 25°C, Dreisbach 1955)

Molar Volume (cm³/mol):
- 304.6 (20°C, calculated-density)
- 384.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
- 9.36 (RP-HPLC-k′ correlation, Sherblom et al. 1992)

Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):

Fugacity Ratio at 25°C, \(F\):
- 1.0

Water Solubility (g/m³ or mg/L at 25°C):
- 0.233 (vapor saturation-shake flask-GC, Sherblom et al. 1992)
- 0.233, 0.0885, 0.181 (calculated-\(V_m\), \(K_{\text{OW}}\), 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°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)

Henry’s Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
- 9.36 (RP-HPLC-k′ correlation, Sherblom et al. 1992)

Octanol/Air Partition Coefficient, log \(K_{\text{O\Lambda}}\):

Bioconcentration Factor, log BCF or log \(K_{\text{B}}\):

Sorption Partition Coefficient, log \(K_{\text{OC}}\):
Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_{\frac{1}{2}} \):
Half-Lives in the Environment:

**TABLE 3.1.33.1**
 Reported vapor pressures of tridecylbenzene at various temperatures

<table>
<thead>
<tr>
<th>Zwolinski &amp; Wilhoit 1971</th>
<th>Kasehgari et al. 1993</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>( P/Pa )</td>
</tr>
<tr>
<td>193</td>
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<td>5333</td>
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<td>7999</td>
</tr>
<tr>
<td>251</td>
<td>10666</td>
</tr>
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<td>271.6</td>
<td>19998</td>
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<tr>
<td>283.1</td>
<td>26664</td>
</tr>
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</tr>
<tr>
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<td>321.3</td>
<td>66661</td>
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<td>329.8</td>
<td>79993</td>
</tr>
<tr>
<td>337.2</td>
<td>93326</td>
</tr>
</tbody>
</table>
3.1.1.34 Tetradecylbenzene

Common Name: Tetradecylbenzene
Synonym: 1-phenyltetradecane
Chemical Name: \( n \)-tetradecylbenzene
CAS Registry No: 1459-10-5
Molecular Formula: \( C_{20}H_{34}, C_6H_5(CH_2)_{13}CH_3 \)
Molecular Weight: 274.484
Melting Point (°C): 16 (Dreisbach 1955; Lide 2003)
Boiling Point (°C): 359 (Dreisbach 1955; Lide 2003)
Density (g/cm³): 0.8549, 0.8514 (20°C, 25°C, Dreisbach 1955)
Molar Volume (cm³/mol): 321.7 (20°C, calculated-density)
406.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
1333* (205°C, derived from compiled data, temp range 205–354°C, Zwolinski & Wilhoit 1971)
0.0055 (extrapolated-Antoine eq., Dreisbach 1955; quoted, Sherblom et al. 1992)
\[ \log (P/mmHg) = 7.56143 - 2522.8/(180.0 + t/°C); \text{ temp range 235–410°C (Antoine eq. for liquid state, Dreisbach 1955)} \]
\[ \log (P/mmHg) = 7.101 - 2042/(130 + t/°C); \text{ temp range 205–300°C (Antoine eq., Zwolinski & Wilhoit 1971)} \]
0.002 (P L, GC-RT correlation, Sherblom et al. 1992)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \( K_{\text{ OW}} \):
9.95 (RP-HPLC-k’ correlation, Sherblom et al. 1992)

Octanol/Air Partition Coefficient, log \( K_{\text{ OA}} \):

Bioconcentration Factor, log BCF or log \( K_{\text{ B}} \):

Sorption Partition Coefficient, log \( K_{\text{ OC}} \):

Environmental Fate Rate Constants, k, and Half-Lives, \( t_{\frac{1}{2}} \):

Half-Lives in the Environment:
### TABLE 3.1.1.34.1
Reported vapor pressures of tetradecylbenzene at various temperatures

**Zwolinski & Wilhoit 1971**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<td>353</td>
<td>98659</td>
</tr>
<tr>
<td>233</td>
<td>4000</td>
<td>354</td>
<td>101325</td>
</tr>
<tr>
<td>241</td>
<td>5333</td>
<td></td>
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<tr>
<td>248</td>
<td>6666</td>
<td></td>
<td></td>
</tr>
<tr>
<td>254</td>
<td>7999</td>
<td>eq. 2</td>
<td>P/mmHg</td>
</tr>
<tr>
<td>263</td>
<td>10666</td>
<td>A</td>
<td>7.010</td>
</tr>
<tr>
<td>270</td>
<td>13332</td>
<td>B</td>
<td>2042.0</td>
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<tr>
<td>285</td>
<td>19998</td>
<td>C</td>
<td>130.0</td>
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<td>295</td>
<td>26664</td>
<td></td>
<td></td>
</tr>
<tr>
<td>304</td>
<td>33331</td>
<td>bp/°C</td>
<td>354.0</td>
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<tr>
<td>312</td>
<td>39997</td>
<td>ΔH_v/(kJ mol⁻¹)</td>
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</tr>
<tr>
<td>324</td>
<td>53329</td>
<td>at 25°C</td>
<td>99.6</td>
</tr>
<tr>
<td>334</td>
<td>66661</td>
<td>at bp</td>
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<tr>
<td>350</td>
<td>93326</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### 3.1.1.35 Styrene

![Styrene structure](image)

**Common Name:** Styrene  
**Synonyms:** phenylethene, styrol, styrole cinnamene, cinnamol, phenylethylene, vinylbenzene, ethenylbenzene  
**Chemical Name:** styrene  
**CAS Registry No:** 100-42-5  
**Molecular Formula:** C₈H₈, C₆H₅CH=CH₂  
**Molecular Weight:** 104.150

**Melting Point (°C):**  
- –30.65 (Lide 2003)

**Boiling Point (°C):**  
- 145 (Lide 2003)

**Density (g/cm³ at 20°C):**  
- 0.9060, 0.9012 (20°C, 25°C, Dreisbach & Martin 1949; Dreisbach 1955; Riddick et al. 1986)  
- 0.906 (Weast 1982–83)

**Molar Volume (cm³/mol):**  
- 115.0 (20°C, calculated-density)  
- 133.0 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Vaporization, ∆Hᵥ (kJ/mol):**  
- 43.932, 38.7 (25°C, bp, Riddick et al. 1986)

**Enthalpy of Fusion, ∆Hₕ (kJ/mol):**  
- 10.95 (Riddick et al. 1986; Chickos et al. 1999)

**Entropy of Fusion, ∆Sₕ (J/mol K):**  
- 45.15, 52.2 (exptl., calculated-group additivity method, Chickos et al. 1999)

**Fugacity Ratio at 25°C, F:** 1.0

**Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**  
- 330* (24°C, shake flask-Karl Fischer titration, measured range 7–51°C, Lane 1946)  
- 310* (cloud point method, measured range 10–60°C, Lane 1946)  
- 220 (shake flask-method not specified, Frilette & Hohenstein 1948)  
- 300 (shake flask-UV, Andrews & Keefer 1950)  
- 160 (shake flask-UV, Frilette & Hohenstein 1948)  
- 250* (recommended best value, temp range 10–60°C, Shaw 1989b)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):**  
- 288* (8.2°C, mercury manometer, measured range –7.7 to 8.2°C, Linder 1931)  
- log (P/mmHg) = 7.929 – 2103/(T/K); temp range 33.5–116.3°C (isoteniscope method, Burchfield 1942)  
- 841.3* (static-Hg manometer, measured range 12.5–60°C, Pitzer et al. 1946)  
- 969.4* (calculated-Antoine eq. regression, Stull 1947)  
- log (P/mmHg) = 7.22302 – 1629.2/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

**Notes:**  
- ln x = –19.471 – 1655.9/(T/K) – 4.6244 × 10⁻⁵·(T/K)²; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
log (P/mmHg) = 8.2696 – 2221.21/(T/K); temp range 32.4–82.9°C (Chaiyavech & van Winkle 1959)

log (P/mmHg) = [–0.2185 × 9634.7/(T/K)] + 7.922049; temp range –7.0 to 145.2°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = 7.14016 – 1574.51/(224.087 + t/°C); temp range 32.4–62.19°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)

log (P/mmHg) = 7.06623 – 1507.434/(214.985 + t/°C); temp range 29.92–144.77°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/atm) = (1 – 418.675/T) × 10^(0.886470 – 8.14267 × 10^-4·T + 7.57896 × 10^-7·T^2); T in K, temp range 281.35–417.92 K (Cox vapor pressure eq., Chao et al. 1983)

log (P/mmHg) = 55.8621 – 4.024 × 10^3/(T/K) – 17.609·log (T/K) + 6.6842 × 10^-3·(T/K) + 1.9438 × 10^-13·(T/K)^2, temp range 243–648 K (Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°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 (20°C, selected from reported experimental determined values, Staudinger & Roberts 1996, 2001)

log K_{AW} = 5.628 – 1935/(T/K) (summary of literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{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 K_{OA}:

Bioconcentration Factor, log BCF:

1.13 (goldfish, Ogata et al. 1984)

Sorption Partition Coefficient, log K_{OC}:

3.42–2.74 (Swann et al. 1983)

2.96, 2.71 (quoted exptl., calculated-MCI χ, Meylan et al. 1992)

Environmental Fate Rate Constants, k, and Half-Lives, t_1/2:

Volatilization: Volatilization and biodegradation may be dominant transport and transformation processes for styrene in water; calculated volatilization t_1/2 = 3 h from a river 1-m deep with a current speed of 1.0 m/s and wind velocity of 3 m/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, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{O3} = 1.8 \times 10^4 \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with ozone at 30°C (Bufalini & Altshuller 1965)
$k_{O3} = (22.6 \pm 4.6) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (relative rate method, Atkinson et al. 1982)
$k_{OH} = 5.25 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1985)
$k_{O3} = (22 \pm 0.014) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH} = (5.87 \pm 0.15) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO3} = (1.51 \pm 0.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson & Aschmann 1988)
$k_{OH} = 5.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: $t_{1/2}$(aerobic) = 336–672 h, based on unacclimated grab samples of aerobic soil and a subsurface sample; $t_{1/2}$(anaerobic) = 1344–2688 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 (Fu & Alexander 1992) $t_{1/2}$(aerobic) = 14 d, $t_{1/2} = 56$ d in natural waters (Capel & Larson 1995)

Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants or Half-Lives:

Half-Lives in the Environment:
Air: atmospheric $t_{1/2} \sim 2.4$–24 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 $t_{1/2}$(calc) = 2.5 h, the reaction $t_{1/2} = 3.5$ h with OH radicals and $t_{1/2} = 9$ h with ozone (Howard 1989);
photooxidation $t_{1/2} = 0.9$ to 7.3 h, based on measured rate data for the reaction with OH radical and O$_3$ in air (Howard et al. 1991);
calculated lifetimes of styrene due to reaction with OH radicals, NO$_3$ radicals and O$_3$ are ~3 h, ~4 h and 1 d, respectively, for ambient atmospheric conditions (Tuazon et al. 1993);
calculated lifetimes of 1.4 h, 3.7 h and 1.0 d for reactions with OH radical, NO$_3$ radical and O$_3$ respectively (Atkinson 2000).

Surface water: $t_{1/2} = 0.6$ d in surface waters in case a first order reduction process may be assumed (Zoeteman et al. 1980)
$t_{1/2} = 336$–672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
$t_{1/2}$(calc) = 0.75–51 d for styrene loss from surface waters (Fu & Alexander 1992).

Ground water: $t_{1/2} = 672$–5040 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and acclimated aqueous screening test data (Howard et al. 1991).

Sediment:
Soil: $t_{1/2} = 336$–672 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

<table>
<thead>
<tr>
<th>Lane 1946</th>
<th>Shaw 1989b (IUPAC) recommended values</th>
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<tbody>
<tr>
<td><strong>shake flask-titration</strong></td>
<td><strong>shake flask-cloud pt.</strong></td>
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<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>7</td>
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<td>24</td>
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<td>32</td>
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<td>400</td>
</tr>
<tr>
<td>51</td>
<td>450</td>
</tr>
</tbody>
</table>

| 10 | 290 |
| 20 | 300 |
| 25 | 340 |
| 30 | 340 |
| 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 3.1.35.2
Reported vapor pressures of styrene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\log (T/K) \quad (4)
\end{align*}
\]

1. Linder 1931

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
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<td>–7.7</td>
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<td>59.8</td>
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Burchfield 1942

isoteniscope method

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>eq. 4 P/mmHg</th>
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<td>–30.6</td>
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</table>

data presented by

Clausius-Clapeyron eq.

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/mmHg</th>
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<tbody>
<tr>
<td></td>
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</tr>
</tbody>
</table>

measured temp range:

33.5–116.3°C

\[\Delta H_\text{ fus}(kJ \text{ mol}^{-1}) = 10.95\]

2. Dreyer et al. 1955

Chaiyavech & Van Winkle 1959

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
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<tbody>
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<td>32.4</td>
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<tr>
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<td>1827</td>
<td>35.6</td>
<td>2666</td>
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<td>74.42</td>
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<td>56877</td>
<td>82.9</td>
<td>13332</td>
</tr>
</tbody>
</table>

\[\Delta H_\text{v}(kJ \text{ mol}^{-1}) = 43.93\] at 25°C

\[\Delta \text{Hv}(kJ \text{ mol}^{-1}) = 10.95\]
FIGURE 3.1.1.35.2 Logarithm of vapor pressure versus reciprocal temperature for styrene.
3.1.1.36 α-Methylstyrene

Common Name: α-Methylstyrene
Synonym: isopropenylbenzene
Chemical Name: α-Methylstyrene
CAS Registry No: 98-83-9
Molecular Formula: C₉H₁₀, C₆H₅C(CH₃)=CH₂
Molecular Weight: 118.175
Melting Point (°C):
    -23.2 (Lide 2003)
Boiling Point (°C):
    165.4 (Lide 2003)
Density (g/cm³):
    0.9106, 0.9062 (20°C, 25°C, Dreisbach 1955)
    0.9082 (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
    129.8 (20°C, calculated-density)
    155.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘuş (kJ/mol):
    11.92 (Chickos et al. 1999)
Entropy of Fusion, ΔSₘuş (J/mol K):
    47.55, 53.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°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* (7.4°C, summary of literature data, temp range 7.4–165.4°C, Stull 1947)
    log (P/mmHg) = 7.28240 – 1740.3/(230 + t°C) (Antoine eq., Dreisbach & Martin 1949)
    333 (extrapolated by formula., Dreisbach 1855)
    log (P/mmHg) = 6.92366 – 1486.88/(202.4 + t°C); temp range 70–220°C (Antoine eq. for liquid state, Dreisbach 1955)
    log (P/mmHg) = [–0.2185 × 10214.6/(T/K)] + 7.959753; temp range 7.4–165.4°C (Antoine eq., Weast 1972–73)
    log (P/mmHg) = 6.92366 – 1486.88/(202.4 + t°C); temp range not specified (Antoine eq., Dean 1985, 1992)
    log (P/kPa) = 6.04856 – 1486.88/(–70.75 + T/K); temp range 343–493 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
    log (P/kPa) = 6.294 – 1599.88/(–63.72 + T/K); temp range 353–413 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
    log (P/mmHg) = –0.8626 – 2.5638 × 10³/(T/K) + 5.3807·log (T/K) – 1.3516 × 10⁻²·(T/K)², temp range 250–654 K (Yaws 1994)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log Kₐₗₗₚ:
    3.48 (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₐ₉₈:
Bioconcentration Factor, log BCF or log Kᵦ:
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
  Photooxidation: $k = (52 \pm 6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at $298 \pm 2 \text{ K}$ (Atkinson 1989).
- Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

## TABLE 3.1.1.36.1
Reported vapor pressures of α-methylstyrene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>$t/°C$</th>
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<td>165.4</td>
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<td>mp/°C</td>
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</table>

**Stull 1947**

Summary of literature data

**FIGURE 3.1.1.36.1** Logarithm of vapor pressure versus reciprocal temperature for α-methylstyrene.
3.1.1.37 β-Methylstyrene

Common Name: β-Methylstyrene
Synonym: propenylbenzene
Chemical Name: β-Methylstyrene
CAS Registry No: 766-90-5 (cis-); 873-66-5 (trans-)
Molecular Formula: C₉H₁₀, C₆H₅CH=CHCH₃
Molecular Weight: 118.175

Melting Point (°C):
-61.6 (cis-, Stephenson & Malanowski 1987; Lide 2003)
-29.3 (trans-, Stephenson & Malanowski 1987; Lide 2003)

Boiling Point (°C):
174 (cis-, Stephenson & Malanowski 1987)
175–176 (trans-, Stephenson & Malanowski 1987)
167.5 (cis-, Lide 2003)
178.3 (trans-, Lide 2003)

Density (g/cm³):
0.9088 (20°C, cis-, Lide 2003)
0.9023 (25°C, trans-, Lide 2003)

Molar Volume (cm³/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, ΔHₘₐₜ (kJ/mol):

Entropy of Fusion, ΔSₘₐₜ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°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°C, summary of literature data, measured range 32.1–112°C, temp range 17.5–179°C, Stull 1947)
267 (calculated by formula, Dreisbach 1955)

log (P/mmHg) = 6.92339 – 1499.80/(201.0 + t°C); temp range 75–200°C (Antoine eq. for liquid state, Dreisbach 1955)

log (P/mmHg) = (–0.2185 × 10701.3/(T/K)) + 8.071487; temp range 17.5–179°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = 6.92339 – 1499.80/(201.0 + t°C); temp range not specified (Antoine eq., Dean 1985, 1992)

log (Pₖ/kPa) = 6.04829 – 1499.8/(–72.15 + T/K); temp range 348–498 K (cis-, liquid, Antoine eq., Stephenson & Malanowski 1987)

log (Pₖ/kPa) = 6.58873 –1915.94/(–33.996 + T/K); temp range 291–452 K (trans-, liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log Kₐw:

Octanol/Air Partition Coefficient, log Kₐₐ:

Bioconcentration Factor, log BCF or log K₉:

Sorption Partition Coefficient, log Kₘ₉:
Environmental Fate Rate Constant and Half-Lives:

Volatilization:

Photolysis:

Photooxidation: rate constant $k = (59 \pm 6) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for the gas-phase reactions with OH radical at 298 ± 2 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

Half-Lives in the Environment:

<table>
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<tr>
<th>TABLE 3.1.1.37.1</th>
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<tr>
<td><strong>Reported vapor pressures of β-methylstyrene at various temperatures and the coefficients for the vapor pressure equations</strong></td>
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<td>101325</td>
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<tr>
<td>mp/°C</td>
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</table>

**FIGURE 3.1.1.37.1** Logarithm of vapor pressure versus reciprocal temperature for β-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: \( \text{C}_9\text{H}_{10} \), \( 2\text{-CH}_3\text{C}_6\text{H}_4\text{CH}=\text{CH}_2 \)
Molecular Weight: 118.175
Melting Point (°C):
-68.5 (Lide 2003)
Boiling Point (°C):
169.8 (Lide 2003)
Density (g/cm\(^3\)):
0.9106 (20°C, Weast 1982–83)
Molar Volume (cm\(^3\)/mol):
129.8 (20°C, calculated-density)
155.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m\(^3\) or mg/L at 25°C):

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
387* (32.1°C, differential manometer, measured range 32.1–112°C, Clements et al. 1953)
\[ \log (P/\text{mmHg}) = 7.15212 - 1628.405/(211.386 + t/°C); \text{ temp range 32.1–112°C (Antoine eq. from differential manometer measurements, Clements et al. 1953)} \]
240.8 (extrapolated-Antoine eq., Driesbach 1955)
\[ \log (P/\text{mmHg}) = 7.09235 - 1582.7/(206.0 + t/°C); \text{ temp range 75–200°C (Antoine eq. for liquid state, Driesbach 1955)} \]
298.9 (extrapolated-Antoine eq., Boublik et al. 1973)
\[ \log (P/\text{mmHg}) = 7.21287 - 1644.083/(214.585 + t/°C); \text{ temp range 32–112.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)} \]
log (P/atm) = (1 – 443.504/(T/K) × 10\(^4\)[0.890379 – 7.17666 × 10\(^3\)/(T/K) + 5.97058 × 10\(^7\)/(T/K)\(^2\)]; temp range 305.16–385.5 K (Cox vapor pressure eq., Chao et al. 1983)
246.4 (extrapolated-Antoine eq., Boublik et al. 1984)
\[ \log (P/\text{mmHg}) = 6.33107 - 1660.041/(214.219 + t/°C); \text{ temp range 32–112.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]
\[ \log (P/\text{mmHg}) = 7.2129 - 1644.08/(214.59 + t/°C); \text{ temp range 32–112°C (Antoine eq., Dean 1985, 1992)} \]
\[ \log (P/\text{mmHg}) = 6.88461 - 1485.41/(200.0 + t/°C); \text{ temp range 75–255°C (Antoine eq., Dean 1985, 1992)} \]
\[ \log (P/\text{kPa}) = 6.27762 - 1628.405/(–61.764 + T/K); \text{ temp range 305–385 K (liquid, Antoine eq., Stephenson & Malanowski 1987)} \]
\[ \log (P/\text{mmHg}) = 36.8413 - 3.7269 \times 10^9/(T/K) - 9.7997 \log (T/K) + 1.4115 \times 10^{-10}(T/K) + 1.9658 \times 10^{-4}(T/K)^2; \text{ temp range 200–659 K (Yaws 1994)} \]

Henry’s Law Constant (Pa·m\(^3\)/mol):
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 3.1.1.38.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of o-methylstyrene at various temperatures</td>
</tr>
<tr>
<td>Clements et al. 1953</td>
</tr>
</tbody>
</table>

<table>
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<th>$t/°C$</th>
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<td>1765</td>
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<td>70.2</td>
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<td>82.8</td>
<td>5529</td>
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<tr>
<td>bp/°C</td>
<td>169.8</td>
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</tbody>
</table>

$\Delta H_f = 35.54 \text{ kJ/mol}$

$\log P = A - B/(C + t/°C)$

<table>
<thead>
<tr>
<th>eq. 2</th>
<th>mmHg</th>
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</thead>
<tbody>
<tr>
<td>A</td>
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<tr>
<td>B</td>
<td>1628.405</td>
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<tr>
<td>C</td>
<td>211.386</td>
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</tbody>
</table>

**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: C₉H₁₀, 3-CH₃C₆H₄CH=CH₂
Molecular Weight: 118.175
Melting Point (°C):
-86.3  (Lide 2003)
Boiling Point (°C):
164  (Lide 2003)
Density (g/cm³ at 20°C):
0.9028  (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
130.9  ((20°C, calculated-density)
155.2  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
2693*  (67.6°C, mercury manometer, measured range 67.6–169.1°C, Buck et al. 1949)
\( \log (P/\text{mmHg}) = -3563/(T/\text{K}) - 7.553\log (T/\text{K}) + 30.90; \) temp range 80–120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
687*  (41.48°C, differential manometer, Clements et al. 1953)
\( \log (P/\text{mmHg}) = 6.95079 - 1520.412/(210.967 + t/°C); \) temp range 41.48–111.8°C (Antoine eq. from differential manometer measurements, measured range 41.48–111.8°C, Clements et al. 1953)
257  (calculated by formula, Dreisbach 1955)
\( \log (P/\text{mmHg}) = 6.99468 - 1553.4/(206.0 + t/°C); \) temp range 75–225°C (Antoine eq. for liquid state, Dreisbach 1955)
228, 244  (extrapolated-Antoine eq., Boublík et al. 1973)
\( \log (P/\text{mmHg}) = 7.06423 - 1564.74/(204.083 + t/°C); \) temp range 67.6–169°C (Antoine eq. from reported exptl. data, Boublík et al. 1973)
\( \log (P/\text{mmHg}) = 7.11224 - 1615.091/(210.809 + t/°C); \) temp range 41.7–111.8°C (Antoine eq. from reported exptl. data, Boublík et al. 1973)
\( \log (P/\text{atm}) = (1 - 442.985/T) \times 10^8((0.888561 - 7.19653 \times 10^{-7}T + 6.75359 \times 10^{-6}T^2); \) T in K, temp range 314.93–442.15 K (Cox vapor pressure eq., Chao et al. 1983)
227, 244  (extrapolated-Antoine eq., Boublík et al. 1984)
\( \log (P/\text{kPa}) = 6.17253 - 1553.744/(202.922 + t/°C); \) temp range 67.6–169.1°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
\( \log (P/\text{kPa}) = 6.22823 - 1609.825/(210.331 + t/°C); \) temp range 41.7–111.8°C (Antoine eq. from reported exptl. data, Boublík et al. 1984)
\( \log (P/\text{mmHg}) = 7.27534 - 1695.4/(220.0 + t/°C); \) temp range 10–72°C (Antoine eq., Dean 1985, 1992)
\( \log (P/\text{mmHg}) = 6.87928 - 1471.28/(200.0 + t/°C); \) temp range 72–250°C (Antoine eq., Dean 1985, 1992)
Mononuclear Aromatic Hydrocarbons

245 (Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P_j/kPa) = 6.07569 - 1520.412/(71.183 + T/K); \text{ temp range } 314-385 \text{ K} \ (\text{Antoine eq., Stephenson & Malanowski 1987})
\]

\[
\log (P/\text{mmHg}) = 11.6959 - 2.9912 \times 10^3/(T/K) + 0.33334 \log (T/K) - 8.8935 \times 10^{-3} \times (T/K) + 4.9793 \times 10^{-6} \times (T/K)^2,
\]

\text{temp range } 187-657 \text{ K} \ (\text{Yaws 1994})

Henry’s Law Constant (Pa m^3/mol at 25°C):

387 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log \(K_{ow}\):

3.35 (Leo et al. 1971)

Octanol/Air Partition Coefficient, log \(K_{oa}\):

Bioconcentration Factor, log \(BCF\):

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 \(K_{oc}\):

Environmental Fate Rate Constants, \(k\), and Half-Lives, \(t_{1/2}\):

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 3.1.1.39.1</th>
</tr>
</thead>
</table>

Reported vapor pressures of \(-m\)-methylstyrene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - B/(T/K) \quad (1)
\]

\[
\ln P = A - B/(T/K) \quad (1a)
\]

\[
\log P = A - B/(C + t/°C) \quad (2)
\]

\[
\ln P = A - B/(C + t/°C) \quad (2a)
\]

\[
\log P = A - B/(C + T/K) \quad (3)
\]

\[
\log P = A - B/(T/K) - C \log (T/K) \quad (4)
\]

**Buck et al. 1949**

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**Clements et al. 1953**

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<td>71.01</td>
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<td>77.12</td>
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</tbody>
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\(\Delta H_v = 38.79 \text{ kJ/mol}\)

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FIGURE 3.1.1.39.1 Logarithm of vapor pressure versus reciprocal temperature for \( m \)-methylstyrne.
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: C₉H₁₀, 4-CH₃C₆H₄CH=CH₂
Molecular Weight: 118.17
Melting Point (°C):
  –34.1  (Lide 2003)
Boiling Point (°C):
  172.8  (Lide 2003)
Density (g/cm³ at 20°C):
  0.9016, 0.9060  (20°C, 25°C, Dreisbach 1955)
  0.8760  (20°C, Weast 1982–83)
Molar Volume (cm³/mol):
  129.8  (20°C, calculated-density)
  155.2  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
  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°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*  (16°C, summary of literature data, temp range 16–175°C, Stull 1947)
  2773*  (68.6°C, mercury manometer, measured range 68.6–170°C, Buck et al. 1949)
  log (P/mmHg) = −3476/(T/K) − 6.923·log (T/K) + 29.03; temp range 80–120°C (vapor pressure eq. from Hg manometer measurements, Buck et al. 1949)
  log (P/mmHg) = 7.34046 − 1791.0/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)
  log (P/mmHg) = 376* (31.82°C, differential manometer, measured range 31.8–96.9°C, Clements et al. 1953)
  log (P/mmHg) = 7.0483 − 1594.7/(209.889 + t/°C); temp range 31.8–96.9°C (Antoine eq. from differential manometer measurements, Clements et al. 1953)
  241.5  (calculated by formula, Dreisbach 1955)
  log (P/mmHg) = 7.35420 − 1765.6/(223.8 + t/°C); temp range 75–205°C (Antoine eq. for liquid state, Dreisbach 1955)
  log (P/mmHg) = [−0.2185 × 10724.2/(T/K)] + 8.130903; temp range 16.0–175°C (Antoine eq., Weast 1972–73)
  216.6, 241  (extrapolated-Antoine eq., Boublik et al. 1973)
  log (P/mmHg) = 7.01119 − 1535.073/(200.732 + t/°C); temp range 68.6–170°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
  log (P/mmHg) = 6.11531 − 1591.082/(209.441 + t/°C); temp range 31.8–96.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
  log (P/atm) = (1 − 443.748/(T/K) × 10^4[0.875061 − 7.08160 × 10^4(T/K) + 7.33467 × 10^7(T/K)^2]; temp range: 289.15–443.15 K, (Cox vapor pressure eq., Chao et al. 1983)
  215, 241  (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 6.11531 – 1521.514/(199.299 + t°C); temp range 68.6–170°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.16144 – 1586.596/(209.046 + t°C); temp range 31.8–96.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.0112 – 1535.1/(200.7 + t°C); temp range 68–170°C (Antoine eq., Dean 1985, 1992)

(242 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 50.6506 – 4.0628 × 10³/(T/K) – 15.524·log (T/K) + 5.5381 × 10–3·(T/K) – 1.1313 × 10–13·(T/K)², temp range 239–665 K (Yaws 1994)

Henry’s Law Constant (Pa m³/mol at 25°C):

287 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K<sub>OW</sub>:

3.35 (Leo et al. 1971; quoted, Ogata et al. 1984)

Octanol/Air Partition Coefficient, log K<sub>OA</sub>:

Bioconcentration Factor, log BCF:

1.55 (gold fish, flow-through method, Ogata et al. 1984)

1.55, 1.62 (gold fish, quoted, calculated-MCI 𝜇, Ogata et al. 1984)

Sorption Partition Coefficient, log K<sub>OC</sub>:

Environmental Fate Rate Constants, k, and Half-Lives, t<sub>½</sub>:

Half-Lives in the Environment:

**TABLE 3.1.1.40.1**

Reported vapor pressures of phenylmethylstyrene at various temperatures and the coefficients for the vapor pressure equations

<table>
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<th>T/°C</th>
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<th>T/°C</th>
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### TABLE 3.1.1.40.1 (Continued)

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<th>Stull 1947</th>
<th>Buck et al. 1949</th>
<th>Dreisbach &amp; Shrader 1949</th>
<th>Clements et al. 1953</th>
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<td><strong>summary of literature data</strong></td>
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<td><strong>differential manometer</strong></td>
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<td>$t/°C$</td>
<td>$P/\text{Pa}$</td>
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<td>mp/°C</td>
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<td>eq. 4</td>
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<td>B</td>
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<td>C</td>
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<td>bp/°C</td>
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<td>$\Delta H_v$</td>
<td>38.95 kJ/mol</td>
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</table>

**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: C_{10}H_{12}
Molecular Weight: 132.202
Melting Point (°C):
–35.7 (Lide 2003)
Boiling Point (°C):
207.6 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
0.9702 (20°C, Weast 1982–83; Dean 1985)
0.9695, 0.9660 (20°C, 25°C, Riddick et al. 1986)
Molar Volume (cm³/mol):
136.4 (20°C, calculated-density)
177.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):
12.477 (Riddick et al. 1986)
12.45 (Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):
52.44, 49.6 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
14.94 (calculated-QSAR Data base, Passino & Smith 1987)

Vapor Pressure (Pa at 25°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°C, temp range 93.8–171.06°C, Herz & Schufan 1922)
53.3* (mercury manometer, measured range –2.4–65°C, Linder 1931)
66.66* (39.3°C, ebulliometry, measured range 39.3–148.6°C, Gardner & Brewer 1937)
133.3* (38°C, summary of literature data, temp range 38–207°C, Stull 1947)

\[
\log (P/\text{mmHg}) = \left[-0.2185 \times 11613.0/(T/\text{K})\right] + 8.194951; \text{ temp range 38–207.2°C (Antoine eq., Weast 1972–73)}
\]

\[
\log (P/\text{mmHg}) = \left[1– 480.364/(T/\text{K})\right] \times 10^4\{0.85916 – 5.75417 \times 10^{-4}/(T/\text{K}) + 4.41971 \times 10^{-3}/(T/\text{K})^2\}; \text{ temp range 311.15–710.93 K, (Cox eq., Chao et al. 1983)}
\]
53.75 (extrapolated-Antoine eq., Dean 1985, 1992)

\[
\log (P/\text{mmHg}) = \text{7.07055 – 1741.30/(208.26 + u°C)}; \text{ temp range 94–206°C (Antoine eq., Dean 1985, 1992)}
\]
53.0 (selected lit. average, Riddick et al. 1986)

\[
\log (P/\text{kPa}) = \text{11.079 – 2797.90/(T/K) + 1.187-log (T/K)}, \text{ temp range not specified (Antoine eq., Riddick et al. 1986)}
\]
56.7 (Antoine eq., extrapolated, Stephenson & Malanowski 1987)

\[
\log (P/\text{kPa}) = \text{6.35719 – 1854.82/(–54.237 + T/K)}; \text{ temp range 311–481 K (Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log (P/\text{mmHg}) = \text{39.9174 – 4.132 \times 10^3/(T/K) – 10.78-log (T/K) + 1.9691 \times 10^{-10}/(T/K) + 2.0405 \times 10^{-6}/(T/K)^2}, \text{ temp range 237–720 K (Yaws 1994)}
\]
38.35* (20.26°C, static method, measured range 253.8–442.8 K, Mokbel et al. 1998)
Henry’s Law Constant (Pa m³/mol at 25°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 (0, 15, 20, 25, 30°C, EPICS-GC, Ashworth et al. 1988)

\[ \ln \left[ \frac{H}{(\text{atm m}^3 \text{ mol}^{-1})} \right] = 11.83 - \frac{5392}{(T/K)} \] temp range 10–30°C (EPICS-GC, Ashworth et al. 1988)

142.8 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

\[ \log K_{AW} = 6.332 - 2215/(T/K) \] (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{OW} \):

3.83 (calculated-fragment const., Rekker 1977)

Octanol/Air Partition Coefficient, log \( K_{OA} \):

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), and Half-Lives, \( t_\frac{1}{2} \):

Volatilization:

Photolysis:

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO₃ radical and \( k_{O_3} \) with O₃ or as indicated, *data at other temperatures see reference:

\[ k_{OH} = (3.43 \pm 0.06) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]
\[ k_{NO_3} = (8.6 \pm 1.3) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at room temp. (relative rate method, Atkinson & Aschmann 1988)

\[ k_{OH} = 3.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (recommended, Atkinson 1990)

\[ k_{OH}(\text{calc}) = 11.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \]
\[ k_{OH}(\text{exptl}) = 34.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (SAR [structure-activity relationship], Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) 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

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\log P = A - \frac{B}{C + T/K} \quad (2) \\
\log P = A - \frac{B}{C + t/°C} \quad (3) \\
\log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\]

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<tr>
<th>Temperature (°C)</th>
<th>Vapor Pressure (Pa)</th>
<th>Source</th>
</tr>
</thead>
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<tr>
<td>93.8</td>
<td>2666</td>
<td>Herz &amp; Schuftan 1922</td>
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<td>103</td>
<td>4000</td>
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<td>140</td>
<td>15732</td>
<td>Gardner &amp; Brewer 1937</td>
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<td>150</td>
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FIGURE 3.1.1.41.1 Logarithm of vapor pressure versus reciprocal temperature for tetralin.

Tetralin: vapor pressure vs. 1/T

- experimental data
- Stull 1947

b.p. = 207.6 °C
### 3.2 SUMMARY TABLES AND QSPR PLOTS

#### TABLE 3.2.1
Summary of the physical properties of mononuclear aromatic hydrocarbons

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<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>mp °C</th>
<th>bp °C</th>
<th>Fugacity ratio, F at 25 °C*</th>
<th>Density, ρ g/cm³ at 20°C</th>
<th>Molar volume, Vm cm³/mol</th>
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* Assuming ΔS_{sub} = 56 J/mol K.

# at 25°C.
TABLE 3.2.2
Summary of selected physical-chemical properties of mononuclear aromatic hydrocarbons at 25°C

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<th>Compound</th>
<th>P^0/Pa</th>
<th>P^1/Pa</th>
<th>S/(g/m^3)</th>
<th>C^2/(mol/m^3)</th>
<th>C^3/(mol/m^3)</th>
<th>log K_{OW}</th>
<th>H/(Pa·m^3/mol) calculated P/C</th>
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### TABLE 3.2.3
Suggested half-life classes of mononuclear aromatic hydrocarbons in various environmental compartments at 25°C

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where,

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<tr>
<td>2</td>
<td>17 (~ 1 day)</td>
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<td>3</td>
<td>55 (~ 2 days)</td>
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<td>4</td>
<td>170 (~ 1 week)</td>
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<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
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<td>6</td>
<td>1700 (~ 2 months)</td>
<td>1,000–3,000</td>
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<td>7</td>
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<td>3,000–10,000</td>
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<td>8</td>
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<td>9</td>
<td>55000 (~ 6 years)</td>
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**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.
3.3 REFERENCES


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Sangster, J. (1993) LOGKOW databank. Sangster Research Laboratory, Montreal, Q.C.


4 Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

4.1 List of Chemicals and Data Compilations

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4.1.2 Chlorinated polynuclear aromatic hydrocarbons

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4.1.3 Polychlorinated naphthalenes

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4.1.4 Brominated polynuclear 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: C9H10
Molecular Weight: 118.175
Melting Point (°C):
-51.38 (Lide 2003)
Boiling Point (°C):
177.97 (Lide 2003)
Density (g/cm³ at 20°C):
0.9639 (Weast 1982–83; Dean 1985; Lide 2003)
Molar Volume (cm³/mol):
123.0 (20°C, calculated-density)
143.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Evaporation, \( \Delta H_v \) (kJ/mol):
49 ± 1.5 (Ambrose & Sprake 1976)
Enthalpy of Fusion, \( \Delta H_{fus} \) (kJ/mol):
8.60 (exptl., Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fus} \) (J/mol K):
38.77, 45.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
5523* (91.68°C, ebulliometry, measured range 91.68–129.05°C, Stull et al. 1961)
204.0* (comparative ebulliometry, extrapolated from vapor pressure equation derived from exptl data, Ambrose & Sprake 1976)

\[
\log (P/kPa) = 6.10462 - 1574.160/(T/K) - 67.079; \text{ temp range 355.006–482.437 K } \text{ (vapor pressure eq., ebulliometry, Ambrose & Sprake 1976)}
\]


\[
\log (P/\text{atm}) = [1 - 451.051/(T/K)] \times 10^8 \times (0.859420 - 6.08324 \times 10^{-4} \times (T/K)) + 4.77502 \times 10^{-7} \times (T/K)^2; \text{ temp range 355.01–452.24 K } \text{ (Cox eq., Chao et al. 1983)}
\]

195.6 (extrapolated-Antoine eq., Boublík et al. 1984)

\[
\log (P/kPa) = 6.1012 - 1571.723/(205.798 + t/°C); \text{ temp range 81.86–209.3°C } \text{ (Antoine eq. from reported exptl. data of Ambrose & Sprake 1976, Boublík et al. 1984)}
\]

196.9 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

\[
\log (P/kPa) = 6.11622 - 1580.315/(–66.49 + T/K); \text{ temp range 374–466 K } \text{ (Antoine eq., Stephenson & Malanowski 1987)}
\]

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \( K_{OW} \):

- 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 \( K_{OA} \):

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{OC} \):

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_{1/2} \):

Volatileization:
- Photolysis: photolysis rate \( k < 3 \times 10^{-5} \) s\(^{-1}\) with \( t_{1/2} > 1 \) d (Kwok et al. 1997)
- Oxidation: rate constant \( k \) for gas-phase second-order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO3} \) with NO\(_3\) radical and \( k_{O3} \) with O\(_3\) or as indicated; *data at other temperatures see reference:
  - \( k_{OH} = 9.2 \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) at 295 K (Atkinson 1989)
  - \( k_{OH}(exptl) = (19 \pm 5) \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\), \( k_{OH}(calc) = 8.3 \times 10^{-12} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) with a calculated lifetime of 8 h; \( k_{NO3}(exptl) = (6.6 \pm 2.0) \times 10^{-15} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) with a calculated lifetime of 7 d; and \( k_{O3}(exptl) < 3 \times 10^{-19} \) cm\(^3\) molecule\(^{-1}\) s\(^{-1}\) with a calculated lifetime of > 55 d at 297 ± 2 K (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
- Air: photolysis \( t_{1/2} > 1 \) d; calculated tropospheric lifetimes of 8 h, 7 d and > 55 d due to reactions with OH radical, NO\(_3\) radical and 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

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<th>( \log P = A - B/(T/K) )</th>
<th>( \ln P = A - B/(T/K) )</th>
<th>( \log P = A - B/(C + t/°C) )</th>
<th>( \ln P = A - B/(C + t/°C) )</th>
<th>( \log P = A - B/(C + T/K) )</th>
<th>( \log P = A - B/(T/K) - C \cdot \log (T/K) )</th>
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<td>( t/°C )</td>
<td>( P/Pa )</td>
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<td>91.68</td>
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<td>176.03</td>
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<td>9860</td>
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(Continued)
### TABLE 4.1.1.1 (Continued)

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<td>t/°C</td>
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<td>mp/K</td>
<td>221.77</td>
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<td>ΔH_{fus}/(kJ mol⁻¹) = 8.60</td>
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<tr>
<td>B</td>
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<td>ΔH_v/(kJ mol⁻¹) = 39.67</td>
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<td>451.12 K</td>
<td>at 298.15 K</td>
<td>49.0</td>
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<tr>
<td>ΔH_v/(kJ mol⁻¹) = 39.8 at bp</td>
<td></td>
<td>49.0</td>
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<tr>
<td>ΔH_v/(kJ mol⁻¹) = 49.0 at 298.15 K</td>
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<td>eq. 3</td>
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<td>C</td>
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#### FIGURE 4.1.1.1

Logarithm of vapor pressure versus reciprocal temperature for indan.

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### Naphthalene

- **Common Name:** Naphthalene
- **Synonym:** naphthene, tar camphor, moth balls
- **Chemical Name:** naphthalene
- **CAS Registry No:** 91-20-3
- **Molecular Formula:** C_{10}H_{8}
- **Molecular Weight:** 128.171
- **Melting Point (°C):** 80.26 (Lide 2003)
- **Boiling Point (°C):** 217.9 (Lide 2003)
- **Density (g/cm³ at 20°C):** 1.0253 (Weast 1983–84)
- **Molar Volume (cm³/mol):**
  - 125.0 (20°C, calculated-from density)
  - 133.2 (from density, Bohon & Claussen 1951)
  - 147.6 (calculated-Le Bas method at normal boiling point)
- **Enthalpy of Vaporization, ΔH_v (kJ/mol):**
- **Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):**
  - 73.93 (Colomina et al. 1982)
  - 72.92 (Van Ekeren et al. 1983)
- **Enthalpy of Fusion, ΔH_{fus} (kJ/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, ΔS_{fus} (J/mol 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°C (assuming ΔS_{fus} = 56 J/mol K), F:** 0.287 (mp at 80.26°C)
  - 0.310 (calculated, Passivirta et al. 1999)

#### Water Solubility (g/m³ or mg/L at 25°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°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°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 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)
- 31.2* (shake flask-UV, measured range 29–73.4°C, Wauchope & Getzen 1972)

- \[ \text{R} \times \text{n} = \frac{-8690}{(T/K)} + (0.000408) [(T/K) - 291.15]^2 - 13.4 + 0.0139(T/K); \text{ temp range 29.2–73.4°C (shake flask-UV, Wauchope & Getzen 1972)} \]

- 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* (25°C, shake flask-fluorescence, measured range 8–31°C, Schwarz & Wasik 1977)
31.69 (generator column-HPLC/UV, measured temp range 5–30°C, May et al. 1978)

S/(mg/kg) = 13.66 + 0.2499·(t/°C) + 0.0189·(t/°C)^2; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978)

30.64 (generator column-HPLC/UV, Wasik et al. 1983)


R·ln x = –80.55/(θ/K) + 28.7/[1/(θ/K) – 1/(T/K)] + 0.31·{[(θ/K)/(T/K)] – 1 – ln [(θ/K)/(T/K)]}, θ = 298.15 K, temp range 8.2–27°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* (25°C, shake flask-UV, Bennett & Canady 1984)

ln x = –1767.4601/R · (T/K) + (17.95209/R) · ln (T/K) + 1; temp range 2–45°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)

33.71* (shake flask-UV, measured range 5–40°C, Perez-Tejeda et al. 1990)

log [S/(mol/dm^3)] = –31.24 – 143.5/(T/K) + 4.772·ln (T/K); temp range 5–40°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)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

log (P/mmHg) = 7.091 – 3465/(T/K); temp range 87–224 (static isotenoscope method, Mortimer & Murphy 1923)

log (P/mmHg) = 29.820/(T/K) – 200.682·log (T/K) + 595.642; measured temp range 10–30°C (effusion, Swan & Mack 1925)

log (P/mmHg) = 10.40 – 3429/(T/K); temp range 15–33°C (effusion, Zil'berman-Granovskaya 1940)

log (P/mmHg) = –[108.30/(t/°C + 27)] + 1.115; temp range 19–35°C (manometry-Rodebuch gauge, Sears & Hopke 1949)

10.8* (effusion method, measured range 6.7–20.7°C, Bradley & Cleasby 1953)

log (P/cmHg) = 10.597 – 3783/(T/K); temp range 6.7–20.7°C, (Antoine eq., effusion, Bradley & Cleasby 1953)

6815* (126.325°C, manometry, measured range 126.3–218.6°C, Camin & Rossini 1955)

log (P/mmHg) = 6.84577 – 1606.529/(187.227 + t/°C); temp range 126.3–218.6°C (Antoine eq. Camin & Rossini 1955)

log (P/mmHg) = 10.75 – 3616/(T/K); temp range –20 to 10°C (Knudsen effusion method, Hoyer & Peperle 1958)

0.1188* (–13°C, Knudsen effusion, measured range –43 to –13°C, Miller 1963)

46.66* (40.33°C, Hg manometer, measured range 40.33–80.34°C, Fowler et al. 1968)

10.98, 32.95 (manometry, extrapolated solid, supercooled liquid P_d, Fowler et al. 1968)

log (P_d/mmHg) = 9.58102 – 2692.92/(t/°C + 220.651); temp range 40–80°C (Antoine eq., mercury manometer, Fowler et al. 1968)

log (P_d/mmHg) = 7.03382 – 1756.91/(t/°C + 204.931); temp range 81–180°C (Antoine eq., mercury manometer, Fowler et al. 1968)

30.66* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)

log (P_d/mmHg) = 7.01065 – 1733.71/(201.859 + t/°C); temp range 86.581–250.27°C (Antoine eq., Zwolinski & Wilhoit 1971)

11.60 (interpolated-Antoine eq., Weast 1972–73)

log (P_d/mmHg) = –[0.2185 × 17065.2/(T/K)] + 11.450; temp range 0–80.0°C (Antoine eq., Weast 1972–73)

log (P_d/mmHg) = [–0.2185 × 1231.16/(T/K)] + 8.413089; temp range 52.6–217.9°C (Antoine eq., Weast 1972–73)

12.26* (Knudsen effusion method, extrapolated from measured data, Radchenko & Kitagorodskii 1974)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

\[ \log (P/\text{mmHg}) = 11.7041 - 3796.574/(T/K); \text{ temp range 9.0–23.91°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)} \]

10.93* (gas saturation, Sinke 1974)

11.21* (Baratron model diaphragm pressure gauge, Ambrose et al. 1975)

\[ \log (P/Pa) = 12.675 - 3796.574/(T/K); \text{ temp range 9.0–23.91°C (Antoine eq., Knudsen effusion, Radchenko & Kitiagorodskii 1974)} \]

13.5 (effusion method-pressure gauge, DePablo 1976)

10.64* (gas saturation, interpolated-Clapeyron eq., Macknick & Prausnitz 1979)

\[ \log (P/\text{Pa}) = 14.501 - 3861.8/(T/K); \text{ temp range 271.46–284.63 K (Antoine eq., Knudsen effusion, Colomina et al. 1982)} \]

11.33* (gas saturation-GC, Grayson & Fosbraey 1982)

\[ \log (P/Pa) = 12.675 - 3796.574/(T/K); \text{ temp range 253–273 K (torsion effusion, regression, de Kruif 1980)} \]

11.41* (gas saturation-GC, Grayson & Fosbraey 1982)

\[ \log (P/Pa) = 12.675 - 3796.574/(T/K); \text{ temp range 253–273 K (weighing effusion, regression, de Kruif 1980)} \]

10.42* (gas saturation-GC, Grayson & Fosbraey 1982)

\[ \log (P/Pa) = 12.675 - 3796.574/(T/K); \text{ temp range 253–273 K (effusion, mean regression, de Kruif 1980)} \]

11.41* (gas saturation-GC, Grayson & Fosbraey 1982)

\[ \log (P/Pa) = 12.675 - 3796.574/(T/K); \text{ temp range 253–273 K (effusion, mean regression, de Kruif 1980)} \]

**Note:** The above equations and values are illustrative and may not be exhaustive. For specific applications, consult the original sources provided in the citations.
log \( (P/T)_{	ext{mmHg}} \) = 2.25180 – 76.496/(–25.09 + t°C); temp range 80.16–90.15°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 \( P_L \) values converted from literature \( P_S \) with different \( \Delta S_{\text{ fus}} \) values, Hinckley et al. 1990)

0.7634* (0°C, gas saturation-GC, measured range –30.6 to 0°C, Wania et al. 1994)

log \( (P/P_{\text{Pa}}) \) = 13.93 – 3851/(T/K); temp range –30 to 0°C, (Antoine eq., gas saturation, Wania et al. 1994)

24.0 (supercooled liquid \( P_L \), 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 \( P_S \), van der Linde et al. 1998)

40.0; 12.4 (quoted \( P_S \) from Hinckley et al. 1990; converted to \( P_S \) with fugacity ratio F, Passivirta et al. 1999)

log \( (P/P_{\text{Pa}}) \) = 10.90 – 2927/(T/K) (solid, Passivirta et al. 1999)

log \( (P/P_{\text{Pa}}) \) = 8.06 – 1923/(T/K) (supercooled liquid, Passivirta et al. 1999)

log \( (P/P_{\text{Pa}}) \) = 13.59 – 3742/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

37.0 (supercooled liquid \( P_L \), GC-RT correlation, Lei et al. 2002)

log \( (P/P_{\text{Pa}}) \) = –2930/(T/K) + 11.39; \( \Delta H_{\text{vap.}} \) = –56.1 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)

Henry’s Law Constant (Pa m³/mol at 25°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 (20°C, 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°C, Alaee et al. 1996)

ln \( K_{\text{AW}} \) = 13.95 – 5364.45/(T/K), temp range: 3.7–35.5°C (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 \( K_{\text{AW}} \) = 6.058 – 2332/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \) at 25°C or as indicated:

3.37 (shake flask, Fujita et al. 1964; Hansch et al. 1973)

3.37, 3.01, 3.45 (Leo et al. 1971)

3.37 (calculated-fragment const., Rekker 1977)

3.395 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)

3.30, 3.01, 3.37, 3.45, 3.59 (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 (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)

3.36 (HPLC-k’ correlation, Hafkenscheid & Tomlinson 1983)

3.35; 3.42 (shake flask; ALPM, Garst & Wilson 1984)

3.57 (HPLC-RV correlation, Garst & Wilson 1984)

3.38 (RP-HPLC correlation, Chin et al. 1986)

3.43 (HPLC-RT correlation, Eadsforth 1986)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

3.29 (HPLC-RT correlation, Wang et al. 1986)
3.29 (HPLC-RT correlation, de Kock & Lord 1987)
3.30 (average, HPLC-RT correlation, Ge et al. 1987)
3.35 (shake flask-GC, Oppenhuizen et al. 1987)
3.23 (HPLC-RT correlation, Minick et al. 1988)
3.29 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
3.35 (recommended, Sangster 1989, 1993)
3.49 (centrifugal partition chromatography, Menges et al. 1990)
3.36 (shake flask-HPLC/UV, Menges & Armstrong 1991)
3.30 (TLC-RT correlation, De Voogt et al. 1990)
3.37 (shake flask-UV, pH 7.4, Alcorn et al. 1993)
3.30 (recommended, Hansch et al. 1995)
3.44; 3.68 (26°C; 4°C, quoted, Piatt et al. 1996)
3.47, 3.58; 3.40 (HPLC-RT correlation: ODS column; Diol column; quoted lit. average, Helweg et al. 1997)
3.40 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
3.77 (RP-HPLC-RT correlation, short ODP column, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C:
5.10 (calculated-$K_{OW}/K_{AW}$, Wania & Mackay 1996)
5.19 (calculated-$S_{oct}$ and vapor pressure, P. Abraham et al. 2001)

Bioconcentration Factor, log BCF at 25°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 $K_{OW}$, Mabey et al. 1982)
4.10, 3.84, 4.25 (average, *Selenastrum capricornutum*-dosed singly, dosed simultaneously, Casserly et al. 1983)
2.11; 2.43 (*Chlorella fusca*; calculated-$K_{OW}$, Geyer et al. 1984)
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 $K_{OC}$ at 25°C or as indicated:
3.11 (natural sediment, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979)
2.38 (22°C, 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 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: pH 7.0, 0.69% OC; pH 5.8, 2.24% OC; pH 7.1, 1.12% OC at 0.15–0.5 mm, batch equilibrium-sorption isotherm, Rippen et al. 1982)
3.11; 3.16 (soils: Alfisol 0.76% OC at pH 7.5, Entisol 1.11% 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 χ, Behnack & 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 (15, 25, 35, 50°C, 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: concn ratio C_{sed}/C_{W}; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
3.11 (calculated-MCI 1χ, 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) (4°C, low organic carbon sediment f_{OC} = 0.0002, batch equilibrium; column expl., Piatt et al. 1996)
3.90 (range 3.81–4.00); 2.11 (range 2.11–2.13) (26°C, low organic carbon sediment f_{OC} = 0.0002, batch equilibrium; column expl., Piatt et al. 1996)
3.74 (humic acid, HPLC-k′ correlation; Nielsen et al. 1997)
2.42–2.56 (5 soils, 20°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 ± 0.073 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choju et al. 1998)
2.91, 2.86, 2.88, 2.87, 2.89, 2.95, 3.07; mean 2.88 ± 0.22 (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Choju 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 expl., 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 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
2.91, 3.02, 2.71 (soils: organic carbon OC ≥ 0.1%, OC ≥ 0.5%, 0.1 ≤ OC < 0.5%, average, Delle Site 2001)
3.06 (average values for sediments OC ≥ 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, t_{1/2}:
Volatilization/Evaporation: rate of evaporation estimated to be 1.675 × 10^{-9} mol cm^{-2} h^{-1} at 20°C and air flow rate of 50 L h^{-1} (Gückel et al. 1973);
calculated t_{1/2} = 7.15 h from 1 m depth of water (Mackay & Leinonen 1975; quoted, Haque et al. 1980);
t_{1/2} = 16 h for surface waters for a river 1-m deep, water velocity 0.5 m/s, wind velocity 1m/s (Southworth 1979; Herbes et al. 1980);
evaporation t_{1/2} = 50 h in a river and t_{1/2} = 200 h in a lake when considering current velocity and wind speed in combined with typical reaeration rates for natural bodies of water (Howard 1989);
t_{1/2}(expt) = 28 min and t_{1/2}(calc) = 32 min from solution (Mackay et al. 1983).
Photolysis:
t_{1/2} = 71 h calculated for direct photochemical transformation near-surface water and t_{1/2} = 550 d in 5-m deep inland water body at 40°N at midday of midsummer (Zepp & Schlottzauer 1979)
k = 0.0392 h^{-1} with H_{2}O_{2} under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)
k = 0.028 h^{-1} in distilled water with t_{1/2} = 25 h (Fukuda et al. 1988)
k = 6.0 × 10^{-4} min^{-1} and t_{1/2} = 19.18 h, photodegradation in methanol-water (3:7, v/v) solution with initial concentration of 50.0 ppm by high-pressure mercury lamp or sunlight (Wang et al. 1991);
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

\[ k(\text{exptl}) = 0.000511 \text{ min}^{-1} \] with \( t_{1/2}(\text{calc}) = 22.61 \text{ h} \) and the predicted \( k = 0.000303 \text{ min}^{-1} \) by QSPR, the pseudo-first-order direct photolysis rate constant of in aqueous solution when irradiated with a 500W medium pressure mercury lamp (Chen et al. 1996)

\[ t_{1/2}(\text{calc}) = 15.42 \text{ h} \] direct photolysis half-life in atmospheric aerosol (QSPR, Chen et al. 2001).

Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with \text{OH} \) radical, \( k_{\text{NO}_3} \) with \text{NO}_3 \) radical and \( k_{\text{O}_3} \) with \text{O}_3 \) or as indicated; *data at other temperatures and/or Arrhenius equation see reference:

\[ k(\text{calc}) < 360 \text{ M}^{-1} \text{ h}^{-1} \] for singlet oxygen, \( k(\text{calc}) < 1 \text{ M}^{-1} \text{ h}^{-1} \) for peroxy radical (Mabey et al. 1982)

\[ k_{\text{OH}} = (2.42 \pm 0.19) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] with an estimated atmospheric lifetime \( \tau \sim 1 \text{d} \), and \( k_{\text{O}_3} < 2 \times 10^{-9} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) due to night-time reaction with \text{N}_2\text{O}_5 \) in atmosphere (relative rate method, Pitts et al. 1985)

\[ k_{\text{OH}} = (2.17 \pm 0.19) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K (relative rate method, Atkinson & Aschmann 1989)

\[ k_{\text{OH}} = (2.39 \pm 0.09) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K, with a calculated tropospheric lifetime of 5.8 h using a global tropospheric 12-h daytime average \text{OH} \) radical concentration of 2.0 \times 10^6 \text{ molecule cm}^{-3} \) (relative rate method, Phousongphouang & Arey 2002)

Hydrolysis: not hydrolyzable (Mabey et al. 1982).

Biodegradation:

k = 4 \times 10^{-6} \text{ g L}^{-1} \text{ d}^{-1} \text{ ultimate loss process (Lee & Ryan, 1976)}

k = (0.04 – 3.3) \times 10^{-6} \text{ g L}^{-1} \text{ d}^{-1} \text{ (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)

k = 0.04 – 3 \mu \text{g/L d} \text{ for microorganisms (Callahan et al. 1979)}

\( t_{1/2} = 1.9 \text{ d} \), 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)

\( t_{1/2}(\text{aerobic}) = 12 \text{ h} \), based on die-away test data for an oil polluted creek (Walker & Colwell 1976)

\( t_{1/2} = 480 \text{ h} \), for an estuarine river (Lee & Ryan 1976).

\( t_{1/2}(\text{anaerobic}) = 25 \text{ d} \) at pH 8 and \( t_{1/2} = 258 \text{ d} \) at pH 5 (Hambrick et al. 1980);

\( t_{1/2} = 1.9 \text{ d} \), in deeper and slower moving contaminated water (Herbes 1981; Wakeham et al. 1983)

k = 0.23 \text{ h}^{-1} \text{ (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)

k = 3.2 \times 10^{-3} \text{ h}^{-1} \text{ with } t_{1/2} = 9 \text{ h}; k = 7.6 \times 10^{-2} \text{ h}^{-1} \text{ with } t_{1/2} = 9 \text{ h} \text{ for mixed bacterial populations in water and sediment from the same stream (NRCC 1983)}

k = 0.14 \text{ h}^{-1} \text{ with } t_{1/2} = 5 \text{ h}; k < 4 \times 10^{-4} \text{ h}^{-1} \text{ with } t_{1/2} > 72 \text{ d} \text{ 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 mg/L in groundwater from hazardous waste site (Lee et al. 1984)

k = 0.024 \text{ d}^{-1} \text{ with } t_{1/2} = 28 \text{ d} \text{ in groundwater with nutrients and acclimated microbes, k = 0.013 d}^{-1} \text{ with } t_{1/2} = 53 \text{ d} \text{ in river water with acclimated microbes, and k = 0.018 d}^{-1} \text{ with } t_{1/2} = 39 \text{ d} \text{ in river water with nutrients and acclimated microbes (Vaishnav & Babeu 1987)}
k = 0.337 d⁻¹ with t½ = 2.1 d for Kidman sandy loam and k = 0.308 d⁻¹ with t½ = 2.2 d for McLaurin sandy loam all at –0.33 bar soil moisture (Park et al. 1990)
t½(aerobic) = 12–480 h, based on die-away test data and for estuarine river (Howard et al. 1991)
t½(anaerobic) = 500–6192 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 creosote-contaminated 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 × 10⁻⁷ ml cell⁻¹ h⁻¹ (Mabey et al. 1982).
Bioconcentration, Uptake (k₁) or Elimination (k₂) Rate Constants:
k₁ = 197 h⁻¹; k₂ = 1.667 h⁻¹ (Daphnia pulex, Southworth et al. 1978; quoted, Hawker & Connell 1986)
log k₂ = –0.70, –1.70 d⁻¹ (fish, calculated-KOW, Thomann 1989)

Half-Lives in the Environment:
Air: volatility of 2.28 × 10⁴ s (experimental), 7.7 × 10³ s (calculated) for depth of water body of 22.5 m (23°C, Klöpffer et al. 1982);
estimated lifetime of ~1d due to reaction with photochemically produced hydroxyl radical, assuming an average daytime atmospheric OH radical concn of ~1 × 10⁶ molecule/cm³ (Atkinson et al. 1984, 1987; quoted, Howard 1989);
calculated lifetime of ~11 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 N₂O₅ can be calculated to range from ~4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);
t½ = 2.96–29.6 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: t½ = 16 h (calculated for river water 1 m deep, water velocity 0.5 m/s, wind velocity 1 m/s from air-water partition coefficients (Southworth 1979; Hallett & Brecher 1984)
t½ = 71 h of photolysis in near surface water, but t½ = 550 d for a depth of 5 m (calculated from surface water in midsummer at 40°N latitude, Zepf & Schlotzhauer 1979);
calculated t½ = 7.15 h, based on evaporative loss for a water depth of 1 m at 25°C (Mackay & Leinonen 1975); an overall t½ = 2.3 d in Rhine river based on monitoring data (Zoeteman et al. 1980)
in coastal seawater mesocosm experiments: k = 0.058 d⁻¹ with t½ = 12 d in winter at 3–7°C during the periods when volatilization dominates, k = 0.061 d⁻¹ with t½ = 11.3 h with HgCl₂ as poison and k = 0.896 d⁻¹ corresponding to t½ = 0.8 h without poison (Wakeham et al. 1983);
t½ = 12–480 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); photolysis t½ = 22.81 h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater: estimated t½ = 0.6 yr in the Netherlands (Zoeteman et al. 1981);
t½ = 24–6193 h based on estimated unacclimated aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).
Sediment: t½ = 4.9 h in oil contaminated sediment and t½ > 88 d in uncontaminated sediments (Herbes & Schwall 1978; quoted, Howard 1989);
desorption k = 0.031 d⁻¹ with t½ = 21.3 d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
Soil: an overall t½ = 3.6 months in a solid waste site (Zoeteman et al. 1981);
t½ = 0.12–125 d (Sims & Overcash 1983);
t½ = 12 d for both 5 mg/kg and 50 mg/kg added (Bulman et al. 1987);
t½ > 50 d (Ryan et al. 1988);
t½ > 80 d (Howard 1989);
biodegradation k = 0.337 d⁻¹ with t½ = 2.1 d for Kidman sandy loam soil and k = 0.308 d⁻¹ with t½ = 2.2 d for McLaurin sandy loam soil (Park et al. 1990);
t½ = 398–1152 h, based on soil-die-away test data (Howard et al. 1991); t½ = 0.02–46 wk, t½ < 2.1 yr (quoted, Ludington soil, Wild et al. 1991).
Biota: elimination half-lives t½ = 2 d from Oyster for naphthalenes, t½ = 2.0 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

\[ R \ln x = -\Delta H_{\text{fus}}/(T/K) + (0.000408)\{(T/K) - 291.15\}^2 - c + b(T/K) \]  
(1)

\[ S/(\mu g/kg) = a t^3 + b t^{1/2} + c t + d \]  
(2)

\[ R \ln x = -30.55/\theta + 28.7/(1/\theta - 1/T) + 0.31[\theta(T -1 - \ln(\theta/T))] \]  
(3)

\[ \ln x = 1767.460/(R \cdot (T/K)) + (17.95209/R) \cdot \ln (T/K) + 1 \]  
(4)

\[ \log (S/mol.dm^{-3}) = -31.24 - 143.5/(T/K) + 4.772 \cdot \ln (T/K) \]  
(5)

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ΔH_{\text{sol}}/(kJ mol⁻¹)

| 2°C | 4.14 | 64.5 | 166 | temp dependence eq. 1 |
| 7°C | 5.77 | 64.5 | 151 | ln x mole fraction |
| 12°C | 7.24 | 157 | 10²·b | 1.39 ± 0.05 |
| 17°C | 8.49 | 240 | 10²·b | 1.39 ± 0.05 |
| 22°C | 10.17 | 73.4 | 244 | 13.4 ± 0.2 |
| 27°C | 12.80 | 73.4 | 247 | 13.4 ± 0.2 |
| 32°C | 14.23 | ΔH_{\text{fus}}/(kJ mol⁻¹) = 36.36 |
| 37°C | 15.69 | | | |

(Continued)
TABLE 4.1.1.2.1 (Continued)

2. Schwarz & Wasik 1977  

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3. Bennet & Canady 1984  

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FIGURE 4.1.1.2.1 Logarithm of mole fraction solubility (ln 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

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Swan & Mack 1925  
Stull 1947  
Sears & Hopke 1949  
Bradley & Cleasby 1953

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| \( t/°C \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) | \( T/K \) | \( P/Pa \) | \( t/°C \) | \( P/Pa \) | \( eq. 1 \) | \( P/\text{mmHg} \) | \( A \) | \( B \) | \( C \) |
| –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          | eq. 1 \( P/\text{mmHg} \) | A 7.0163 |
| 80.28              | 999.8       | 23.91            | 112.6                    | 293.25         | 6.95          | B 1733.71         | 8575               |
|                    | eq. 1 \( P/Pa \) | 25              | 12.26*                   | 298.26         | 11.35         | C 201.859         |                    |
|                    | A 13.83     | \( \Delta H_{\text{subl}/kJ \text{ mol}^{-1}} = 72.72 \) | 308.17         | 28.95         | eq. 1 \( P/\text{mmHg} \) |                 |
|                    | B 3817      | at 25°C          | 313.24                    | 44.73          | A 26.25       | 303.29             | 18.45              |
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4.

de Kruif 1980
de Kruif et al. 1981

torsion-effusion
diaphragm gauge
torsion-effusion
diaphragm gauge

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5. Colomina et al. 1982

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\[ \Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 72.8 \]

at 25°C

6. Sato et al. 1986

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\[ \Delta H_{\text{subl}}/\text{kJ mol}^{-1} = 73.7 \]

\[ (\text{–30 to 0°C}) \]

\[ eq. 1 \]

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TABLE 4.1.1.2.2 (Continued)

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For solid

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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

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(Continued)
TABLE 4.1.1.2.3 (Continued)

Alaee et al. 1996

gas stripping-GC

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enthalpy of volatilization:
\[ \Delta H_{\text{vol}}/(kJ\cdot\text{mol}^{-1}) = 44.6 \text{ at } 20°C \]

\[ \ln K_{\text{AW}} = A - \frac{B}{(T/\text{K})} \]

eq. 1

\[ K_{\text{AW}} \]

\[ A = -5364.4 \]

\[ B = 13.95 \]

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:** α-methylnaphthalene
- **Chemical Name:** 1-methylnaphthalene
- **CAS Registry No:** 90-12-0
- **Molecular Formula:** C\textsubscript{11}H\textsubscript{10}
- **Molecular Weight:** 142.197

**Melting Point (°C):**
- -30.43 (Lide 2003)

**Boiling Point (°C):**
- 244.7 (Lide 2003)

**Density (g/cm\textsuperscript{3} at 20°C):**
- 1.02015, 1.01649 (20°C, 25°C, Dreisbach 1955)
- 1.0125 (Dean 1985)
- 1.0202 (Lide 2003)

**Molar Volume (cm\textsuperscript{3}/mol):**
- 139.4 (20°C, calculated-density)
- 169.8 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Vaporization, ΔH\textsubscript{v} (kJ/mol):**
- 60.06, 45.48 (25°C, bp, Dreisbach 1955)

**Enthalpy of Fusion, ΔH\textsubscript{fus} (kJ/mol):**
- 4.853 (Dean 1985)
- 4.98, 6.95; 11.92 (−32.45, 34.25°C, total phase change enthalpy, Chickos et al. 1999)

**Entropy of Fusion, ΔS\textsubscript{fus} (J/mol K):**
- 20.69, 28.82 (−32.45, 34.25°C, 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°C, F:** 1.0

**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°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°C, Schwarz & Wasik 1977)
- 29.5* (shake flask-fluorescence, measured range 10−25°C, Schwarz 1977)
- 31.7 (generator column-HPLC, Wasik et al. 1983)
- 27.02 (average lit. value, Pearlman et al. 1984)
- 30.2* (20°C, shake flask-GC, measured range 20–70°C, Burris & MacIntyre 1986)
- 28.0 (recommended, IUPAC Solubility Data Series, Shaw 1989)

**Vapor Pressure (Pa at 25°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)
- \( \log (P/\text{mmHg}) = 7.03592 − 1826.948/(195.002 + t°\text{C}); \) temp range 142.1−254.4°C (Antoine eq., Hg manometer, Camin & Rossini 1955)
- 8.95 (calculated by formula, Dreisbach 1955)
- \( \log (P/\text{mmHg}) = 7.06899 − 1852.674/(197.716 + t°\text{C}); \) temp range 130−305°C (Antoine eq. for liquid state, Dreisbach 1955)
- 66.66* (52.8°C, Hg manometer, measured range 52.8–243.0°C, Myers & Fenske 1955)
- 7.19* (interpolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.03592 – 1826.948/(195.002 + t°C); temp range 107.68–278.32°C (liquid, Antoine eq., Zwolinski & Wilhoit 1971)

8.82* (gas saturation-GC, Macknick & Prausnitz 1979)

8.84 (extrapolated-Clapeyron eq., Macknick & Prausnitz 1979)

log (P/mmHg) = 20.552 – 6933.2/(T/K); temp range 5.70–38.6°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)

7221* (151.15°C, differential pressure gauge, measured range 151.15–271.70°C, Wieczorek & Kobayashi 1981)

log (P/atm) = [1 – 517.727/(T/K)] × 10^{0.863323 – 5.85750 × 10^{-2}(T/K)^2}; temp range 278.85–593.38 K (Cox eq., Chao et al. 1983)

8.84 (interpolated Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.15971 – 1825.586/(194.848 + t°C); temp range: 142.1–245.3°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)

log (P/mmHg) = 7.03592 – 1826.946/(195.0 + t°C); temp range 108–278°C (Antoine eq., Dean 1985, 1992)

0.895 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

log (P/kPa) = 7.03469 – 3006.467/(T/K); temp range 278–313 K (Antoine eq., Stephenson & Malanowski 1987)

8.93* (pressure gauge, interpolated-Antoine eq. derived from exptl. data, temp range –14.44 to + 115°C, Sasse et al. 1988)

log (P/mmHg) = 7.27126 – 2006.662/(212.625 + t°C); temp range –14.44 to115.1°C. (Antoine eq., pressure gauge, Sasse et al. 1998)

7.43 (P_GC by GC-RT correlation with eicosane as reference standard, Hinckley et la. 1990)

log (P/mmHg) = 29.8895 – 3.9535 × 10^3/(T/K) – 7.2253·log (T/K) + 1.1109 × 10^{-11}·(T/K)^3; temp range 243–722 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 (P/kPa) = 6.39609 – 2006.662/(T/K) – 60.525; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

6.55; 1.28 (supercooled liquid P_L: calibrated GC-RT correlation, GC-RT correlation, Lei et al. 2002)

log (P/Po) = –3258/(T/K) + 11.74; ∆H_vap. = –62.4 kJ·mol –1 (GC-RT correlation, Lei et al. 2002)

8.85* (24.05°C, transpiration method, measured range 294.1–324.2 K, Verevkin 2003)

ln (P/Po) = 298.831/R – 83537.555/R·(T/K) – (78.6/R)·ln[(T/K)/298.15]; where P* = 101.325 kPa, gas constant R = 8.31451 J·K^{-1}·mol^{-1} (vapor pressure eq. from transpiration measurements, temp range 294.1–324.2 K, Verevkin 2003)

Henry’s Law Constant (Pa m^3/mol at 25°C) 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°C, Bamford et al. 1999)

ln K_{AW} = –5821.5/(T/K) + 15.636; ∆H = 48.4 kJ mol^{-1}; measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, log K_{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)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

3.33, 3.06 (Lula aquifer 0.032% OC, Apalachic 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; $t_{1/2}$:

Volatile:

Photolysis: calculated $t_{1/2} = 22$ h for direct sunlight photolysis of 50% conversion at 40°N latitude of midday in midsummer in near surface water, $t_{1/2} = 180$ d in 5-m deep inland water and $t_{1/2} = 190$ d in inland water with a suspended sediment concentration of 20 mg/L partitioning (Zepp & Schlotzhauer 1979);

$t_{1/2} = 180$ d under summer sunlight in surface water (Mill & Mabey 1985);

direct photolysis $t_{1/2} = 11.14$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).

Oxidation: rate constant $k$, for gas-phase second-order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$, or as indicated *data at other temperatures see original reference:

$k_{OH} = (5.30 \pm 0.48) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH} < 1.3 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{N_2O_5} = (3.3 \pm 0.7) \times 10^{-17}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with N$_2$O$_5$ at 298 ± 2 K (relative rate method, Atkinson & Aschmann 1987, 1988)

$k_{OH} = 5.30 \times 10^{-11}$ cm$^3$·molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson 1989, 1990)

$k_{OH(calc)} = 59.77 \times 10^{-12}$ cm$^3$·molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{OH} = 5.30 \times 10^{-11}$ cm$^3$·molecule$^{-1}$ s$^{-1}$, $(4.09 \pm 0.20) \times 10^{-11}$ cm$^3$·molecule$^{-1}$ s$^{-1}$ at (298 ± 2)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·cm$^{-3}$ (relative rate method, Phousongphouang & Arey 2002)

Hydrolysis:

Biodegradation: $k = 0.415$ d$^{-1}$ with $t_{1/2} = 1.7$ d for Kidman sandy loam soil and $k = 0.321$ d$^{-1}$ with $t_{1/2} = 2.2$ d for McLaurin sandy loam soil, all at ~3.3 bar soil moisture (Park et al. 1990).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric lifetimes of alkyl-substituted naphthalenes due to reaction with OH radical and with N$_2$O$_5$ calculated to range from ~4 to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987); direct photolysis $t_{1/2} = 11.14$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001); and 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·cm$^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).

Water: computed near-surface $t_{1/2} = 22$ h and for direct photochemical transformation at latitude 40°N, midday, midsummer, and $t_{1/2} = 80$ d with no sediment-water partitioning and $t_{1/2} = 190$ d with sediment-water partitioning for direct photolysis in 5 m deep inland water body integrated over full summer d at latitude 40°N (Zeep & Schlotzhauer 1979);

$t_{1/2} = 180$ d under summer sunlight (Mill & Mabey 1985).

Soil: biodegradation $k = 0.415$ d$^{-1}$ with $t_{1/2} = 1.7$ d for Kidman sandy loam soil, $k = 0.321$ d$^{-1}$ with $t_{1/2} = 2.2$ d for McLaurin sandy loam soil (Park et al. 1990).

Sediment:

Biota: elimination $t_{1/2} = 2$ 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

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<th>t/°C</th>
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</table>

\[ \Delta H_{\text{sol}} / (\text{kJ mol}^{-1}) = 19.1 \]

---

**FIGURE 4.1.1.3.1** Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-methylnaphthalene.
### TABLE 4.1.1.3.2
Reported vapor pressures of 1-methylnaphthalene at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - \frac{B}{T/K} \quad (1) \\
\ln P = A - \frac{B}{T/K} \quad (1a) \\
\log P = A - \frac{B}{C + t/°C} \quad (2) \\
\ln P = A - \frac{B}{C + t/°C} \quad (2a) \\
\log P = A - \frac{B}{C + T/K} \quad (3) \\
\log P = A - \frac{B}{T/K} - C\log (T/K) \quad (4) \\
\ln P/P_{\text{O}} = A - \frac{B}{T/K} - C\ln \left(\frac{T/K}{298.15}\right) \quad (4a)
\]

1.

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<td>240.0</td>
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<td>101325</td>
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<td>ΔH\text{v}/(kJ mol\textsuperscript{-1}) = 46.0</td>
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(Continued)
TABLE 4.1.3.2 (Continued)

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<td>Wieczorek &amp; Kobayashi 81</td>
<td>Sasse et al. 1988</td>
<td>Verevkin 2003</td>
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<tr>
<td>t/°C</td>
<td>t/°C</td>
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<td>B 83537.555/R</td>
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<td>temp range 424–593 K</td>
<td></td>
<td>at 25°C ΔH_v/(kJ mol⁻¹) = 60.7</td>
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FIGURE 4.1.3.2 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

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<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>H/(Pa m³/mol)</th>
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<td>27.8, 30.8</td>
<td>29.2</td>
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<td>25.0</td>
<td>44.8, 51.0</td>
<td>47.8</td>
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<td>31.0</td>
<td>65.7, 78.2</td>
<td>71.7</td>
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</table>

ln \( K_{AW} \) = A – B/(T/K)

A 15.636
B 5821.5

enthalpy, entropy change:
\( \Delta H/(kJ\cdot mol^{-1}) = 48.4 \pm 1.4 \)
\( \Delta S/(J\cdot K^{-1}\cdot mol^{-1}) = 130 \)

at 25°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: \( \text{C}_{11}\text{H}_{10}\)
Molecular Weight: 142.197

Melting Point (°C):
34.6 (Weast 1972–73; Lide 2003)

Boiling Point (°C):

Density (g/cm\(^3\) at 20°C):
1.0058 (Weast 1982–83; Lide 2003)

Molar Volume (cm\(^3\)/mol):
141.4 (20°C, calculated-density)
169.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
59.40, 45.20 (25°, bp, Dreisbach 1955)

Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
11.924 (Parks & Huffman 1931)
5.61, 12.13; 17.74 (15.35, 34.25°C; total phase change enthalpy, Chickos et al. 1999)

Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
39.25 (Tsonopoulos & Prausnitz 1971)
19.43, 39.43 (15.35, 34.25°C, 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°C (assuming \( \Delta S_{\text{ fus}} = 56 \text{ J/mol K} \)), F: 0.805 (mp at 34.6°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C):
24.6 (shake flask-GC, Eganhouse & Calder 1976)
25.4 (shake flask-fluorescence, Mackay & Shiu 1977)
20.0 (Voznáková 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°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 (P/mmHg) = 7.06850 – 1840.268/(198.395 + t°C); temp range 139.1–242°C (Antoine eq., Hg manometer, Camin & Rossini 1955)
10.67 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.06850 – 1840.268/(198.395 + t°C), temp range 130–300°C (Antoine eq. for liquid state, Dreisbach 1955)
9.07* (extrapolated-Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.06850 – 1840.268/(198.395 + t°C); temp range 104.85–274.3°C (Antoine eq., Zwolinski & Wilhoit 1971)
9.07 (extrapolated-Antoine eq., Boublík et al. 1973)
5.60 (20°C, Voznáková et al. 1978)
8629* (151.26°C, differential pressure gauge, measured range 151.26–279.81°C, Wieczorek & Kobayashi 1981)
log (P/atm) = \[1 - 514.242/(T/K)\] \times 10^5[0.879050 - 5.85793 \times 10^{-4}(T/K) + 4.1925 \times 10^{-7}(T/K)^2]; temp range 378.0–629.32 K (Cox eq., Chao et al. 1983)
9.08 (extrapolated-Antoine eq., Boublík et al. 1984)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

\[ \log (P/\text{kPa}) = 6.19638 - 1842.831/(198.692 + t/\degree \text{C}); \text{ temp range 139.2–241.76}\degree \text{C} (\text{Antoine eq. from reported expl. data, Boublik et al. 1984}) \]

6.31 \quad (\text{GC-RT correlation, supercooled liquid, Bidleman 1984})

9.033 \quad (\text{extrapolated, Antoine eq., Dean 1985, 1992})

\[ \log (P/\text{mmHg}) = 7.0685 - 1840.268/(198.4 + t/\degree \text{C}); \text{ temp range 105–274}\degree \text{C} (\text{Antoine eq., Dean 1985, 1992}) \]

9.33 \quad (\text{extrapolated from Antoine eq., Stephenson & Malanowski 1987})

\[ \log (P/\text{kPa}) = 6.21475 - 1858.19/(–72.479 + T/K); \text{ temp range 423–515 K} (\text{Antoine eq., Stephenson & Malanowski 1987}) \]

\[ \log (P/\text{mmHg}) = 56.2052 - 5.2563 \times 10^3/(T/K) - 16.195 \cdot \log (T/K) + 8.1583 \times 10^{-11} \cdot (T/K)^2; \text{ temp range 308–761 K} (\text{vapor pressure eq., Yaws 1994}) \]

Henry’s Law Constant (Pa m³/mol at 25°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 \quad (\text{wetted-wall column-GC, Fendinger & Glotfelty 1990})

50.6 \quad (\text{calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991})

20.265* \quad (26°C EPICS-GC, Hansen et al. 1993)

46.0 \quad (\text{gas stripping-HPLC/fluo., Da Maagd et al. 1998})

62.0 \quad (\text{gas stripping-GC, Altschuh et al. 1999})

51.3* \quad (\text{gas stripping-GC; Bamford et al. 1999})

\[ \ln K_{\text{AW}} = -5099.83/(T/K) + 13.23; \Delta H = 42.4 \text{ kJ mol}^{-1}; \text{ measured range 4.1–31}\degree \text{C} (\text{gas stripping-GC, Bamford et al. 1999}) \]

18620 \quad (20°C, selected value based on Hansen et al. 1993 data, Staudinger & Roberts 1996, 2001)

\[ \log K_{\text{AW}} = 2.245 – 399/(T/K) (\text{van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001}) \]

Octanol/Water Partition Coefficient, log K_{\text{OW}}:

3.864 \quad (\text{shake flask-fluorometry, Krishnamurthy & Wasik 1978})

3.86 \quad (\text{Hansch & Leo 1979})

4.11 \quad (\text{shake flask-UV, concn. ratio, Karickhoff et al. 1979})

3.70 \quad (\text{HPLC-k’ correlation, Hanai et al. 1981})

4.01 \quad (\text{HPLC-RT correlation, Eadsforth 1986})

4.09 \quad (\text{HPLC-RT correlation, Wang et al. 1986})

4.00 \quad (\text{recommended, Sangster 1989})

3.86 \quad (\text{recommended, Hansch et al. 1995})

Bioconcentration Factor, log BCF:

2.61 \quad (\text{quoted from Davies & Dobbs 1984, Sabljic 1987})

2.65 \quad (\text{calculated-MCI } \chi, \text{ Sabljic 1987})

Sorption Partition Coefficient, log K_{\text{OC}}:

3.93 \quad (\text{natural sediments, average sorption isotherms by batch equilibrium technique-UV spec., Karickhoff et al. 1979})

3.40 \quad (\text{sediment 4.02% from Tamar estuary, bath equilibrium-GC, Vowles & Mantoura 1987})

3.719; 3.72; 3.71 \quad (\text{sediment: concn ratio } C_{\text{sed}}/C_{\text{W}}; \text{ 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, t_{1/2}:

- **Vaporization:**
  \[
  k = 0.042 \text{ h}^{-1} \text{ with } t_{1/2} = 6.4 \text{ h} \text{ in distilled water (Fukuda et al. 1988;)}
  \]

- **photolysis:**
  \[
  t_{1/2} = 9.23 \text{ h} \text{ predicted - QSPR, in atmospheric aerosol (Chen et al. 2001).}
  \]

**Hydrolysis:**
Oxidation: rate constant, \( k \) for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with \( \text{O}_3 \) as indicated. *Data at other temperatures see reference:

\[
k_{\text{OH}} = (5.23 \pm 0.42) \times 10^{-11} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \ \text{with a calculated atmospheric lifetime of } \sim 5 \ \text{h, and } \]
\[
k_{\text{O}_3} < 4 \times 10^{-19} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \ \text{at } 295 \pm 1 \ \text{K} \ (\text{relative rate, Atkinson & Aschmann 1986})
\]
\[
k_{\text{NO}_3} = (4.2 \pm 0.9) \times 10^{-17} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \ \text{for reaction with } \text{N}_2\text{O}_5 \text{ at } 298 \pm 2 \ \text{K} \ (\text{relative rate method, Atkinson & Aschmann 1987})
\]
\[
k_{\text{OH}} = 5.23 \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \ \text{at } 298 \ \text{K} \ (\text{Atkinson 1989, 1990})
\]
\[
k_{\text{OH}}(\text{calc}) = 57.36 \times 10^{-12} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \ \text{for reaction with } \text{N}_2\text{O}_5 \text{ at } 298 \ \text{K} \ \text{(relative rate method, Phousongphouang & Arey 2002)}
\]

\[
k_{\text{OH}} = (4.86 \pm 0.25) \times 10^{-11} \ \text{cm}^3 \ \text{molecule}^{-1} \ \text{s}^{-1} \ \text{at } 298 \pm 2 \ \text{K} \ \text{with a calculated tropospheric lifetime to be } 3.4 \ \text{h using a global tropospheric 12-h daytime average OH radical concn of } 2.0 \times 10^6 \ \text{molecule/cm}^3 \ \text{for reaction with OH radical (Phousongphouang & Arey 2002)}.
\]

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:

Air: calculated atmospheric lifetime of \( \sim 4 \ \text{h} \) 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 \( \text{N}_2\text{O}_5 \) can be calculated from \( \sim 4 \) to 13 h and 20–80 d, respectively (Atkinson & Aschmann 1987);

*direct photolysis \( t_\text{halo} = 9.23 \ \text{h} \) (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 \( 2.0 \times 10^6 \ \text{molecule/cm}^3 \) for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water: computed near-surface \( t_\text{halo} = 54 \ \text{h} \) and for direct photochemical transformation at latitude 40°N, midday, midsummer; \( t_\text{halo} = 410 \ \text{d} \) with no sediment-water partitioning and \( t_\text{halo} = 440 \ \text{d} \) with sediment-water partitioning by direct photolysis in a 5-m deep Inland Water Body (Zepp & Schlotzhauer 1979);

*\( t_\text{halo} = 410 \ \text{d} \) under summer sunlight (Mill & Mabey 1985);

*rate constants and half-lives: \( k = 0.064 \ \text{d}^{-1} \), \( t_\text{halo} = 11 \ \text{d} \) in spring at 8–16°C, \( k = 0.687 \ \text{d}^{-1} \), \( t_\text{halo} = 1.0 \ \text{d} \) in summer at 20–22°C, \( k = 0.054 \ \text{d}^{-1} \), \( t_\text{halo} = 13 \ \text{d} \) in winter at 3–7°C for the periods when volatilization appears to dominate, and \( k = 0.046 \ \text{d}^{-1} \), \( t_\text{halo} = 15.1 \ \text{d} \) with \( \text{HgCl}_2 \) as poison, and \( k = 0.954 \ \text{d}^{-1} \), \( t_\text{halo} = 0.7 \ \text{d} \) without poison in September 9–15, in marine mesocosm experiments (Wakeham et al. 1983).

Groundwater:

Sediment:

Soil:

Biota: elimination \( t_\text{halo} = 2 \ \text{d} \) 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

\[
\log P = A - B/(T/K) \quad (1) \\
\log P = A - B/(C + t/°C) \quad (2) \\
\log P = A - B/(C + T/K) \quad (3) \\
\log P = A - B/(T/K) - C\log (T/K) \quad (4)
\]

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<th>Method</th>
<th>Temperature</th>
<th>Pressure (Pa)</th>
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<td><strong>Camin &amp; Rossini 1955</strong></td>
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<td>5536</td>
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<td>150.655</td>
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<td></td>
<td>120.68</td>
<td>2666</td>
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<tr>
<td></td>
<td>130.73</td>
<td>4000</td>
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<td><strong>Wieczorek &amp; Kobayashi 1981</strong></td>
<td>151.26</td>
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### TABLE 4.1.1.4.1 (Continued)

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<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
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<td>eq. 2 P/mmHg</td>
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<td>271.29 188158</td>
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<td>241.052 101325</td>
<td>279.81 221176</td>
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<td>exptl data fitted to</td>
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<td>bp/°C 241.052</td>
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<td>∆H_v/(kJ mol⁻¹) = 46.0</td>
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**FIGURE 4.1.1.4.1** Logarithm of vapor pressure versus reciprocal temperature for 2-methylnaphthalene.
## TABLE 4.1.4.2
Reported Henry’s law constants of 2-methylnaphthalene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ln K_{AW} = A - B/(T/K) )</td>
<td>(1) ( \log K_{AW} = A - B/(T/K) ) (1a)</td>
</tr>
<tr>
<td>( \ln (1/K_{AW}) = A - B/(T/K) )</td>
<td>(2) ( \log (1/K_{AW}) = A - B/(T/K) ) (2a)</td>
</tr>
<tr>
<td>( \ln (k_H/\text{atm}) = A - B/(T/K) )</td>
<td>(3)</td>
</tr>
<tr>
<td>( \ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) )</td>
<td>(4) ( \ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) ) (4a)</td>
</tr>
<tr>
<td>( K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2 )</td>
<td>(5)</td>
</tr>
</tbody>
</table>

### Hansen et al. 1993

<table>
<thead>
<tr>
<th>°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>H/(Pa m³/mol)</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>26.0</td>
<td>20.265</td>
<td>4.1</td>
<td>10.5, 16.2</td>
<td>13.0</td>
<td>7.0 ± 0.14</td>
<td></td>
</tr>
<tr>
<td>35.8</td>
<td>22.900</td>
<td>11.0</td>
<td>18.2, 24.4</td>
<td>21.0</td>
<td>1234 ± 44</td>
<td></td>
</tr>
<tr>
<td>46.0</td>
<td>26.243</td>
<td>18.0</td>
<td>28.8, 38.3</td>
<td>33.2</td>
<td>eq. 4</td>
<td></td>
</tr>
</tbody>
</table>

### Bamford et al. 1999

<table>
<thead>
<tr>
<th>°C</th>
<th>H/(Pa m³/mol)</th>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>H/(Pa m³/mol)</th>
<th>K_{AW}</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>42.1, 62.5</td>
<td>4.1</td>
<td>10.5, 16.2</td>
<td>13.0</td>
<td>13.2307</td>
</tr>
<tr>
<td>31.0</td>
<td>56.2, 95.5</td>
<td>11.0</td>
<td>18.2, 24.4</td>
<td>21.0</td>
<td>5100</td>
</tr>
</tbody>
</table>

### Enthalpy, Entropy Change:

\( \Delta H/(\text{kJ mol}^{-1}) = 42.4 ± 4.2 \)

\( \Delta S/(\text{J mol}^{-1} \text{ K}^{-1}) = 110 \) at 25°C

### FIGURE 4.1.4.2
Logarithm of Henry’s law constant versus reciprocal temperature for 2-methylnaphthalene.
4.1.1.5 1,3-Dimethylnaphthalene

Common Name: 1,3-Dimethylnaphthalene
Synonym:
Chemical Name: 1,3-dimethylnaphthalene
CAS Registry No: 575-41-7
Molecular Formula: C_{12}H_{12}
Molecular Weight: 156.223
Melting Point (°C):
  –6.0 (Weast 1982–83, Dean 1985; Lide 2003)
Boiling Point (°C):
  263 (Dreisbach 1955; Weast 1982–83; Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
  1.0063, 1.0026 (20°C, 25°C, Dreisbach 1955)
  1.0144 (Weast 1982–83; Dean 1985; Lide 2003)
Molar Volume (cm³/mol):
  154.0 (20°C, calculated-density)
  192.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHV (kJ/mol):
  69.58, 48.69 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m³ or mg/L at 25°C):
  8.00 (shake flask-fluorescence, Mackay & Shiu 1977)
  7.81 (average lit. value, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  1.947 (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.0469 – 1845.6/(180.0 + t°C); temp range 150–313°C (Antoine eq. for liquid state, Dreisbach 1955)
log (P/atm) = [1 – 540.353/(T/K)] × 10^{1.72680 – 7.87991 × 10^{-4}·(T/K) + 42.8535 × 10^{-7}·(T/K)^2}; temp range
  400.0–541.0 K (Cox eq., Chao et al. 1983)
  6.950 (interpolated-Antoine eq., Dean 1985, 1992)
  log (P/mmHg) = 7.6347 – 2295.4/(232.4 + t°C); temp range 20–148°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.2698 – 2076.0/(210 + t°C); temp range 148–310°C (Antoine eq., Dean 1985, 1992)
Henry’s Law Constant (Pa m³/mol at 25°C):
  71.03 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, log K_{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 $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\frac{1}{2}$:

Volatileization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$, or as indicated *data at other temperatures see original reference:

$$k_{OH} = (7.49 \pm 0.39) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at (298 \pm 2) K}$$

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 cm$^{-3}$ (relative rate method, Phousongphouang & Arey 2002)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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 cm$^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:
Groundwater:
Sediment:
Soil:

Biota: elimination $t_\frac{1}{2} = 2$ d from Oyster for naphthalenes (quoted, Meador et al. 1995).
4.1.1.6 1,4-Dimethylnaphthalene

Common Name: 1,4-Dimethylnaphthalene
Synonym:
Chemical Name: 1,4-dimethylnaphthalene
CAS Registry No: 571-58-4
Molecular Formula: C\textsubscript{12}H\textsubscript{12}
Molecular Weight: 156.223
Melting Point (°C):
    7.60 (Lide 2003)
Boiling Point (°C):
Density (g/cm\textsuperscript{3} at 20°C):
    1.0166, 1.0129 (20°C, 25°C, Dreisbach 1955)
    1.0166 (Weast 1982–83)
Molar Volume (cm\textsuperscript{3}/mol):
    153.7 (20°C, calculated-density)
    192.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, \( \Delta H_v \) (kJ/mol):
    70.315, 48.62 (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
    10.6 (Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
    37.87, 45.5 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C, F: 1.0
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
    11.4 (shake flask-fluorescence, Mackay & Shiu 1977)
    11.40 (average lit. value, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
    1.55 (calculated by formula, Dreisbach 1955)
    \log (P/mmHg) = 7.0527 – 1869.0/(180.0 + t°C); temp range 155–310°C (Antoine eq. for liquid state, Dreisbach 1955)
    \log (P/mmHg) = 7.6347 – 2345.8/(232.6 + t°C); temp range 20–148°C (Antoine eq., Dean 1985, 1992)
    \log (P/mmHg) = 7.2698 – 2076.0/(210 + t°C); temp range 148–310°C (Antoine eq., Dean 1985, 1992)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):
    48.84 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)
Octanol/Water Partition Coefficient, \( \log K_{\text{OW}} \):
    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, $log K_{OA}$:

Bioconcentration Factor, $log BCF$:

Sorption Partition Coefficient, $log K_{OC}$:

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$, or as indicated *data at other temperatures see original reference:
  $$k_{OH} = (5.79 \pm 0.36) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at (298 \pm 2)K with a calculated tropospheric lifetime ranging from 1.9 to 2.4 h using a global tropospheric 12-h daytime average OH radical concentration of } 2.0 \times 10^6 \text{ molecule cm}^{-3} \text{ (relative rate method, Phousongphouang & Arey 2002)}$$

Hydrolysis:
- Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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 cm$^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).
- Surface water:
- Groundwater:
- Sediment:
- Soil:
- Biota: elimination $t_{1/2} = 2 \text{ d from Oyster for naphthalenes (quoted, Meador et al. 1995).}
4.1.1.7 1,5-Dimethylnaphthalene

Common Name: 1,5-Dimethylnaphthalene
Synonym:
Chemical Name: 1,5-dimethylnaphthalene
CAS Registry No: 571-61-9
Molecular Formula: C_{12}H_{12}
Molecular Weight: 156.223
Melting Point (°C):
   82 (Dreisbach 1955; Weast 1982–83; Lide 2003)
Boiling Point (°C):
   265 (Dreisbach 1955; Weast 1982–83; Lide 2003)
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
   192.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Evaporation, Δ_HV (kJ/mol):
Enthalpy of Fusion, Δ_Hfus (kJ/mol):
Entropy of Fusion, Δ_Sfus (J/mol K):
Fugacity Ratio at 25°C (assuming Δ_Sfus = 56 J/mol K), F: 0.276 (mp at 82°C)
Water Solubility (g/m^3 or mg/L at 25°C):
   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°C or as indicated and reported temperature dependence equations.):
   log (P/mmHg) = 7.0493 – 1855.0/(180.0 + t/°C); temp range 150–313°C (Antoine eq. for liquid state, Dreisbach 1955)
   1.93; 0.513 (supercooled liquid P_L; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
   log (P_P/L = –3346/(T/K) + 11.51; Δ_Hvap. = –64.1 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m^3/mol at 25°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 K_{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 K_{OC}:
Environmental Fate Rate Constants, k, or Half-Lives, t½:
   Volatilization:
   Photolysis:
   Hydrolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$, or as indicated *data at other temperatures see original reference:

$k_{\text{OH}} = (6.01 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(298 \pm 2) \text{ K}$ 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 cm$^{-3}$ (relative rate method, Phousongphouang & Arey 2002).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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 cm$^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 2 \text{ d}$ from Oyster for naphthalenes (quoted, Meador et al. 1995).
4.1.1.8  2,3-Dimethylnaphthalene

Common Name: 2,3-Dimethylnaphthalene
Synonym: guaiene
Chemical Name: 2,3-dimethylnaphthalene
CAS Registry No: 581-40-8
Molecular Formula: C_{12}H_{12}
Molecular Weight: 156.223

Melting Point (°C):
105  (Dreisbach 1955; Weast 1972–73; Lide 2003)

Boiling Point (°C):
268  (Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm³ at 20°C):
1.003  (Weast 1982–83; Lide 2003)

Molar Volume (cm³/mol):
155.8  (20°C, calculated-density)
192.0  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆H_v (kJ/mol):
70.315, 48.97  (25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
25.10  (Ruelle & Kesselring 1997)
15.9  (Chickos et al. 1999)

Entropy of Fusion, ∆S_{fus} (J/mol K):
42.06, 45.5  (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.164 (mp at 105°C)

Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equations):
1.55  (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.0527 − 1869.0/(180.0 + t/°C); temp range 155–315°C (Antoine eq. for liquid state, Dreisbach 1955)
1.86  (extrapolated-Cox eq., Chao et al. 1983)
log (P/atm) = [1– 631.969/(T/K)] × 10^4[1.09999 − 10.2378 × 10^{-4}(T/K) + 11.3931 × 10^{-7}(T/K)^2]; temp range 333.15–408.15 K (Antoine eq.-II, Stephenson & Malanowski 1987)
0.91  (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.27335 − 1383.083/(141.333 + t/°C); temp range 105–135°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
1.543  (interpolated, Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.40396 − 2111.9/(201.1 + t/°C); temp range 20–155°C (Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.0527 − 1869/(180 + t/°C); temp range 155–315°C (Antoine eq., Dean 1985, 1992)
0.437  (Antoine eq., Stephenson & Malanowski 1987)
log (P_{L}/kPa) = 10.635 − 4172.6/(T/K); temp range 278–301 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_{S}/kPa) = 8.97875 − 2959.733/(−59.936 + T/K); temp range 333–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_{L}/kPa) = 5.18084 − 1544.764/(−116.821 + T/K); temp range 378–408 K (Antoine eq.-III, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa m^3/mol at 25°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 K_{ow}:
- 4.396 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)
- 4.40 (Hansch & Leo 1979)
- 4.40 (recommended, Sangster 1993)
- 4.40 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, or Half-Lives, t_1/2:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, all data at other temperatures see reference:

- k_{OH} = \(7.68 \pm 0.48\) \times 10^{-11} cm^3 molecule^{-1} s^{-1}, with a calculated atmospheric lifetime of ~4 h, and
- k_{O_3} < 4 \times 10^{-19} cm^3 molecule^{-1} s^{-1} at 295 \pm 1 K (relative rate method, Atkinson & Aschmann 1986)
- k_{N_2O_5} = (5.7 \pm 1.9) \times 10^{-17} cm^3 molecule^{-1} s^{-1} with N_2O_5 (relative rate method, Atkinson & Aschmann 1987)
- k_{O_3} < 0.4 \times 10^{-18} cm^3 molecule^{-1} s^{-1}, k_{OH} = 7.68 \times 10^{-11} cm^3 molecule^{-1} s^{-1}, k_{N_2O_5} = 5.7 \times 10^{-17} cm^3 molecule^{-1} s^{-1} with N_2O_5 at room temp. (Atkinson & Aschmann 1987, 1988)
- k_{OH} = (76.8 \pm 4.8) \times 10^{-12} cm^3 molecule^{-1} s^{-1} at 295 \pm 1 K (Atkinson 1989)
- k_{OH} = 77 \times 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson 1990)
- k_{OH} = 100.3 \times 10^{-12} cm^3 molecule^{-1} s^{-1} (molecular orbital calculations, Klamt 1996)
- k_{OH} = (6.15 \pm 0.47) \times 10^{-11} cm^3 molecule^{-1} s^{-1} at (298 \pm 2) 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 molecule cm^{-3} (Phousongphouang & Arey 2002)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

- Air: calculated atmospheric lifetime of ~4 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 N_2O_5 can be calculated to range from ~4 to 13 h and 20–80 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 molecule cm^{-3} for the reaction with OH radical (Phousongphouang & Arey 2002).

Surface water:

Groundwater:

Sediment:

Soil:

Biota: elimination t_1/2 = 2 d from Oyster for naphthalenes (quoted, Meador et al. 1995).
4.1.1.9 2,6-Dimethylnaphthalene

Common Name: 2,6-Dimethylnaphthalene
Synonym:
Chemical Name: 2,6-dimethylnaphthalene
CAS Registry No: 581-42-0
Molecular Formula: C_{12}H_{12}
Molecular Weight: 156.223

Melting Point (°C):
112  (Lide 2003)

Boiling Point (°C):
262  (Dreisbach 1955; Dean 1985; Lide 2003)

Density (g/cm³ at 20°C):
1.003, 0.999  (20°C, 25°C, Dreisbach 1955)
1.142  (Dean 1985)

Molar Volume (cm³/mol):
155.8  (calculated-density)
192.0  (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ∆HV (kJ/mol):
69.45, 48.70  (25°C, bp, Dreisbach 1955)

Enthalpy of Fusion, ∆H_{fus} (kJ/mol):
24.27  (Tsonopoulos & Prausnitz 1971)
25.06  (calorimetry, Osborn & Douslin 1975; quoted, Ruelle & Kesselring 1997; Chickos et al. 1999)

Entropy of Fusion, ∆S_{fus} (J/mol K):
63.18  (Tsonopoulos & Prausnitz 1971)
65.39, 45.5  (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming ∆S_{fus} = 56 J/mol K), F: 0.140 (mp at 112°C)

Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equations):
20.41  (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 7.0460 – 1841.0/(180.0 + t/°C); temp range 150–310°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 (P/atm) = [1 – 687.081/(T/K)] × 10^4{1.14901 – 11.9220 × 10^4·(T/K) + 17.3468 × 10^7·(T/K)^2}; temp range 328.15–418.15 K (Cox eq., Chao et al. 1983)
1.41  (extrapolated-Antoine eq., Boublik et al. 1984)
log (P/kPa) = 5.19014 – 1325.209/(139.781 + t/°C); temp range 111–145°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
2.036  (interpolated-Antoine eq., Dean 1985, 1992)
log (P/mmHg) = 7.3968 – 2080.3/(200.8 + t/°C); temp range 20–150°C (Antoine eq., Dean 1992)
log (P/mmHg) = 7.0460 – 1841/(180 + t/°C); temp range 150–310°C (Antoine eq., Dean 1985, 1992)
0.378  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 11.290 – 3047.828/(T/K); temp range 333–368 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/s/kPa) = 8.45107 – 2512.509/(–89.765 + T/K); temp range 384–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/s/kPa) = 5.18084 – 1320.21/(–133.876 + T/K); temp range 384–418 K (Antoine eq.-III, Stephenson & Malanowski 1987)
log (P/mmHg) = –6.9795 – 2.9488 × 10^3/(T/K) + 7.4483·log (T/K) – 1.15821 × 10^-2·(T/K) + 4.3391 × 10^-6·(T/K)^2; temp range 383–777 K (vapor pressure eq., Yaws 1994)

Henry’s Law Constant (Pa m^3/mol at 25°C):
121 (calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, log K_{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 K_{oc}:

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:
Volatilization:
Photolysis: rate constant in distilled water k = 0.045 h^{-1} with t_{1/2} = 15.5 h (Fukuda et al. 1988).
Hydrolysis:
Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3, or as indicated *data at other temperatures see original reference:
k_{OH} = (6.65 ± 0.35) × 10^{-11} cm^3 molecule^{-1} s^{-1} at (298 ± 2) 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 × 10^6 molecule cm^{-3} (relative rate method, Phousongphouang & Arey 2002)
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:
Air: a calculated tropospheric lifetime to be 1.9–2.4 h using a global tropospheric 12-h daytime average OH radical concentration of 2.0 × 10^6 molecule cm^{-3} for the reaction with OH radical (Phousongphouang & Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination t_{1/2} = 2 d from Oyster for naphthalenes (quoted, Meador et al. 1995)
4.1.1.10 1-Ethynaphthalene

Common Name: 1-Ethynaphthalene
Synonym: α-ethynaphthalene
Chemical Name: 1-ethynaphthalene
CAS Registry No: 1127-76-0
Molecular Formula: C₁₂H₁₂
Molecular Weight: 156.223
Melting Point (°C):
  −13.9  (Lide 2003)
Boiling Point (°C):
  258.6  (Lide 2003)
Density (g/cm³ at 20°C):
  1.00816, 1.00446  (20°C, 25°C, Dreisbach 1955)
  1.0082  (Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
  155.0  (20°C, calculated-density)
  192.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔHᵥ (kJ/mol):
  67.42, 46.92  (25°C, bp, Dreisbach 1955)
Enthalpy of Fusion, ΔH₉ₙ (kJ/mol):
Entropy of Fusion, ΔS₉ₙ (J/mol K):
Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°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)
  10.31  (average lit. value, Pearlman et al. 1984)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
  133.3*  (70.0°C, summary of literature data, temp range 70.0–258.1°C, Stull 1947)
  3.0  (calculated by formula, Dreisbach 1955)
log (P/mmHg) = 6.9599 − 1791.4/(180.5 + t/°C); temp range 145–310°C (Antoine eq. for liquid state, Dreisbach 1955)
  2.51*  (extrapolated from liquid state, Antoine eq., Zwolinski & Wilhoit 1971)
log (P/mmHg) = 7.03159 − 1841.320/(185.28 + t/°C); temp range 120–292°C (Antoine eq., Zwolinski & Wilhoit 1971)
log (P/atm) = [1 − 531.480/(T/K)] × 104·(0.923623 − 6.97505 × 10⁻⁴·(T/K) + 5.07450 × 10⁻⁷·(T/K)²); temp range 393.15–565.45 K (Cox eq., Chao et al. 1983)
  2.51  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 6.15645 − 1841.32/(–87.87 + T/K); temp range 393–565 K (Antoine eq., Stephenson & Malanowski 1987
log (P/mmHg) = 7.5650 − 3.7597 × 10³/(T/K) + 2.6035·log (T/K) − 1.1581 × 10⁻²·(T/K) + 5.1365 × 10⁻⁶·(T/K)²; temp range 259–776 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m³/mol at 25°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 $K_{ow}$:
4.39 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)
4.38 (calculated-fragment const., Yalkowsky et al. 1983)
4.42 (calculated-solvatochromic parameters and $V_r$, Kamlet et al. 1988)
4.40 (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 $K_{oa}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{ow}$:
3.77 (sediment, HPLC-$k'$ correlation, Vowles & Mantoura 1987)
3.89 (HPLC-capacity factor correlation, Hodson & Williams 1988)
3.78 (calculated-MCI $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:
Volatilization:
Photolysis:
Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$, or as indicated *data at other temperatures see original reference:

$k_{OH} = (3.64 \pm 0.41) \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at (298 \pm 2)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 cm$^{-3}$ (relative rate method, Phousongphouang & Arey 2002)

Hydrolysis:
Biodegradation:
Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) 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 cm$^{-3}$ for the reaction with OH radical (Phousongphouang & Arey 2002).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1/2} = 2$ d from Oyster for naphthalenes (quoted, Meador et al. 1995).
### TABLE 4.1.1.10.1
Reported aqueous solubilities and vapor pressures of 1-ethynaphthalene at various temperatures

<table>
<thead>
<tr>
<th>Aqueous solubility</th>
<th>Vapor pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Schwarz 1977</strong></td>
<td><strong>Schwarz &amp; Wasik 1977</strong></td>
</tr>
<tr>
<td>shake flask-fluorescence</td>
<td>shake flask-fluorescence</td>
</tr>
<tr>
<td><strong>Schwarz 1977</strong></td>
<td><strong>Schwarz &amp; Wasik 1977</strong></td>
</tr>
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<td>shake flask-fluorescence</td>
<td>shake flask-fluorescence</td>
</tr>
<tr>
<td><strong>Stull 1947</strong></td>
<td><strong>Zwolinski &amp; Wilhoit 1971</strong></td>
</tr>
<tr>
<td>summary of literature data</td>
<td>selected values</td>
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<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
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<tr>
<td>8.6</td>
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<td>31.7</td>
<td>11.72</td>
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\[ \Delta H_{\text{sol}}/(kJ \cdot mol^{-1}) = 14.27 \]

<table>
<thead>
<tr>
<th>mp/°C</th>
<th>( \log P = A - B/(C + t/°C) )</th>
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<tr>
<td>258.1</td>
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<td>259.4</td>
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<td>255.83</td>
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<tr>
<td>260.94</td>
<td>258.94</td>
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</tbody>
</table>

\[ \Delta H_{v}(kJ \cdot mol^{-1}) = \]

at 25°C 48.1

at bp —
FIGURE 4.1.1.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-ethynaphthalene.

FIGURE 4.1.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-ethynaphthalene.
4.1.1.11 2-Ethylnaphthalene

Common Name: 2-Ethylnaphthalene
Synonym: β-ethylnaphthalene
Chemical Name: 2-ethylnaphthalene
CAS Registry No: 939-27-5
Molecular Formula: C_{12}H_{12}
Molecular Weight: 156.223
Melting Point (°C):

-7.4 (Lide 2003)
Boiling Point (°C):

258 (Lide 2003)
Density (g/cm^3 at 20°C):

0.9922 (Weast 1982–83; Lide 2003)
Molar Volume (cm^3/mol):

157.4 (20°C, calculated from density)
192.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, Δ_H_v (kJ/mol):

66.99, 47.33 (25°, bp, Dreisbach 1955)
64.7 (Lei et al. 2002)
Enthalpy of Fusion, Δ_H_fus (kJ/mol):
Entropy of Fusion, Δ_S_fus (J/mol K):
Fugacity Ratio at 25°C), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

7.97 (shake flask-GC, Eganhouse & Calder 1976)
7.97 (average lit. value, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°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 (P/mmHg) = 8.0819 − 1886.0/(191.0 + t°C); temp range 145–300°C (Antoine eq. for liquid state, Dreisbach 1955)
3.24* (extrapolated from liq. state, Antoine eq., Zwolinski & Wilhoit 1971; quoted, Mackay & Shiu 1981)
log (P/mmHg) = 7.07566 − 1880.73/(191.41 + t°C); temp range 119.14–291.9°C (Antoine eq., Zwolinski & Wilhoit 1971)
4.21* (extrapolated exp. data, Macknick & Prausnitz 1979; quoted, Mackay & Shiu 1981)
log (P/mmHg) = 21.485 − 7435.9/(T/K); temp range 13.05–45.1°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
log (P/atm) = [1−531.189/(T/K)] × 10^8×(0.871612 − 5.23140 × 10^−4×(T/K) + 3.70623 × 10^−3×(T/K)^2); temp range 286.2–565.05 K (Cox eq., Chao et al. 1983)
4.21 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_t/kPa) = 7.46683 − 3232.791/(T/K); temp range 286–319 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_t/kPa) = 6.20056 − 1880.73/(−82.74 + T/K); temp range 393–565 K (Antoine eq.-II, Stephenson & Malanowski 1987)
3.71* (pressure gauge in vacuum cell, interpolated-Antoine eq. derived from exp. data, temp range, 4.65–125°C, Sasse et al. 1988)
log (P_t/mmHg) = 6.83511 − 1799.779/(189.505 + t°C); temp range −4.65 to 125.09°C (Antoine eq., pressure gauge, Sasse et al. 1988)
log (P_t/kPa) = 7.46683 − 3232.79/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
2.56; 0.633 (supercooled liquid P_t: calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
log (P_t/Pa) = −3381/(T/K) + 11.75; Δ_H_vap. = −64.7 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol at 25°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 \( K_{ow} \):
- 4.377 (shake flask-fluorometry, Krishnamurthy & Wasik 1978)
- 4.43 (HPLC-k' 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 \( K_{oa} \):
- 3.76 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
- 3.76 (calculated-MCI \( \chi \), Sabljic et al. 1995)

Bioconcentration Factor, log \( BCF \):

Sorption Partition Coefficient, log \( K_{oc} \):
- 3.76 (sediment 4.02% OC from Tamar estuary, batch equilibrium-GC, Vowles & Mantoura 1987)
- 3.76 (calculated-MCI \( \chi \), Sabljic et al. 1995)

Environmental Fate Rate Constants, \( k \), or Half-Lives, \( t_\frac{1}{2} \):
- Volatilization:
  - Photolysis: \( k = 0.038 \text{ h}^{-1} \) in distilled water with \( t_\frac{1}{2} = 18.4 \text{ h} \) (Fukuda et al. 1988).
- Hydrolysis:
- Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with NO\(_3\) radical and \( k_{\text{O}_3} \) with O\(_3\), or as indicated *data at other temperatures see original reference:
  - \( k_{\text{OH}} = (4.02 \pm 0.55) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at \( (298 \pm 2) \text{ K} \) with a calculated tropospheric lifetime to be 3.5 h using a global tropospheric 12-h daytime average OH radical concentration of \( 2.0 \times 10^6 \text{ molecule cm}^{-3} \) (relative rate method, Phousongphouang & Arey 2002)

Biodegradation:
- Biotransformation:
- Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
- Air:
  - Surface water: \( t_\frac{1}{2} = 18.4 \text{ h} \) in distilled water (Fukuda et al. 1988).
- Groundwater:
- Sediment:
- Soil:
- Biota: elimination \( t_\frac{1}{2} = 2 \text{ d} \) from Oyster for naphthalenes (quoted, Meador et al. 1995).

**TABLE 4.1.1.11.1**

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<tr>
<th>Temperature (°C)</th>
<th>Zwolinski &amp; Wilhoit 1971</th>
<th>Macknick &amp; Prausnitz 1979</th>
<th>Sasse et al. 1988</th>
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<td>electronic manometer</td>
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<td>( P )</td>
<td>( t )</td>
<td>( P )</td>
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<td>1333</td>
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TABLE 4.1.1.11.1 (Continued)

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<td>eq. 2</td>
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<td>C</td>
<td>191.41</td>
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<tr>
<td>bp/°C</td>
<td>257.93</td>
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</tr>
<tr>
<td>ΔHv/(kJ mol⁻¹) = 48.1 at bp</td>
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</tr>
</tbody>
</table>

FIGURE 4.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for 2-ethyl naphthalene.
4.1.1.12 1,4,5-Trimethylnaphthalene

Common Name: 1,4,5-Trimethylnaphthalene
Synonym: 
Chemical Name: 1,4,5-trimethylnaphthalene
CAS Registry No: 2131-41-1
Molecular Formula: C13H14
Molecular Weight: 170.250
Melting Point (°C):
   63 (Lide 2003)
Boiling Point (°C):
   285 (Zwolinski & Wilhoit 1971)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
   169.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)
   214.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_fus (kJ/mol): 
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.424 (mp at 63°C)
Water Solubility (g/m³ or mg/L at 25°C):
   2.10 (shake flask-fluorescence, Mackay & Shiu 1977)
   2.04 (average lit. value, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
   0.681 (supercooled liquid P_L, Chao et al. 1983)
   log (P_L/atm) = [1–558.187/(T/K)] × 10^4{0.998467 – 7.03095 × 10⁻¹(T/K) + 1.71801 × 10⁻⁸(T/K)²}; temp range 415.15–558.15 K (Cox eq., Chao et al. 1983)
Henry’s Law Constant (Pa m³/mol at 25°C):
   23.50 (calculated-P/C, Eastcott et al. 1988)
Octanol/Water Partition Coefficient, log K_OW:
   4.90 (calculated-fragment const., Yalkowsky & Valvani 1979, 1980)
   4.79 (calculated-solvability and mp, Mackay et al. 1980)
   4.94 (calculated-solvatochromic parameters and intrinsic molar volume V_i, Kamlet et al. 1988)
   5.10 ± 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 K_OA:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_OC:
Environmental Fate Rate Constants, k, or Half-Lives, t½:
Half-Lives in the Environment:
   Biota: elimination t½ = 2 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: C₁₂H₁₀
Molecular Weight: 154.207
Melting Point (°C):
68.93 (Lide 2003)
Boiling Point (°C):
256.1 (Lide 2003)
Density (g/cm³ at 20°C):
0.866 (Weast 1982–1983)
1.04 (Lide 2003)
Molar Volume (cm³/mol):
148.3 (20°C, calculated-density)
184.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ∆Hₘₜₜ (kJ/mol):
18.58 (Parks & Huffman 1931)
18.66 (exptl., Chickos et al. 1999)
Entropy of Fusion, ∆Sₘₜₜ (J/mol K):
51.05 (Miller et al. 1984)
54.81, 59.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ∆Sₘₜₜ = 56 J/mol K), F: 0.371 (mp at 68.93°C)
0.35 (Mackay et al. 1980, 1983; Shiu & Mackay 1986; Shiu et al. 1987)
0.381 (calculated, ∆Sₘₜₜ = 54 J/mol K, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°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°C, Bohon & Claussen 1951)
3.87 (shake flask-UV, Sahyun 1966)
7.08* (shake flask-UV, measured range 0–64.5°C, Wauchope & Getzen 1972)
R·ln x = −4520/(T/K) + 4.08 × 10⁻⁴·[(T/K) – 298.15]² – 20.8 + 0.0273·(T/K), temp range 24.6–73.4°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)
7.09 (recommended, Pearlman et al. 1984)
7.05 (vapor saturation-UV, Akiyoshi et al. 1987)
6.5 (29°C, 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 [S₀/(mol/L)] = 1.872 −973.4/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = −1.5792 – 3669.26/(T/K), temp range 5–50°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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7933* (162.5°C, isoteniscope-manometer, measured range 162.5–255.2°C, Chipman & Peltier 1929)
104* (69.20°C, temp range 69.20–271.2°C, Cunningham 1930; quoted, Boublik et al. 1984)
133.3* (70.6°C, summary of literature data, temp range 70.6–254.0°C, Stull 1947)
1.30 (effusion method, Bright 1951)

\[
\log (P/mmHg) = 10.38 – 3799/(T/K); \text{ temp range 4.0–34.5°C (Antoine eq., effusion, Bright 1951)}
\]

0.031 (manometry, Augood et al. 1953; selected, Bidleman 1984)
1.273* (effusion method, Bradley & Cleasby 1953; selected, Bidleman 1984; Neely 1983; Erickson 1986)

\[
\log (P/mmHg) = 11.282 – 4263/(T/K); \text{ temp range 15.05–40.55°C (Antoine eq., Bradley & Cleasby 1953)}
\]

5.608 (P L, supercooled liquid converted from literature P S with \( \Delta S_f \) Bidleman 1984)

3.35, 3.41 (P GC by GC-RT correlation with octadecane as reference standard, different columns, BP-1 column, Apolane-87 column, Bidleman 1984)

0.423, 0.703, 0.594 (calculated-MW, GC-RI correlation, calculated-MCI \( \chi \), Burkhard et al. 1985a)

2.03 (supercooled liquid \( P_s \), GC-RI correlation, Burkhard et al. 1985b)

\[
\log (P/mmHg) = 7.24541 – 1998.725/(202.733 + t/°C); \text{ temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\]

1.99 ± 0.03; 1.03, 1.29, 0.579, 0.969 (gas saturation-GC; quoted lit. values Burkhard et al. 1984, 1985b)

1.15* (24.7°C, gas saturation-GC/FID, measured range 5.2–24.7°C, Burkhard et al. 1984)

\[
\log (P/Pa) = 11.05 – 3201/(T/K) (solid, Passivirta et al. 1999)
\]

log (P/kPa) = 6.36895 – 1997.558/(202.608 + t/°C); temp range 69.2–271.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

3.35 (P GC by GC-RT correlation with eicosane as reference standard, different columns, BP-1 column, Apolane-87 column, Bidleman 1984)

0.422–2.54; 2.03–7.04 (quoted range of lit. P S values; lit. P L values, Delle Site 1997)

log (P/L/kPa) = –3265/(T/K) + 11.51; \( \Delta H_{\text{vap.}} = –62.5 \text{ kJ·mol}^{-1} \) (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations):

<table>
<thead>
<tr>
<th>Temperature Dependence</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(gas stripping-GC, Mackay et al. 1979)</td>
<td>41.34</td>
</tr>
<tr>
<td>(gas stripping-GC, Mackay et al. 1980)</td>
<td>30.4</td>
</tr>
<tr>
<td>(gas stripping-GC, Warner et al. 1987)</td>
<td>11.55</td>
</tr>
<tr>
<td>(wetted-wall column-GC, Fendinger &amp; Glotfelty 1990)</td>
<td>19.57</td>
</tr>
<tr>
<td>(calculated-vapor-liquid equilibrium (VLE) data, Yaws et al. 1991)</td>
<td>86.5</td>
</tr>
<tr>
<td>(gas stripping-GC, Shiu &amp; Mackay 1997)</td>
<td>31.20</td>
</tr>
</tbody>
</table>

\[
\log \left[ \frac{H}{\text{Pa m}^3/\text{mol}} \right] = 6.33 - \frac{1255}{T/\text{K}}
\]

(Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log $K_{ow}$:

<table>
<thead>
<tr>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(shake flask-UV, Rogers &amp; Cammarata 1969)</td>
<td>3.16</td>
</tr>
<tr>
<td>(shake flask, Leo et al. 1971; Hansch &amp; Leo 1979)</td>
<td>4.09</td>
</tr>
<tr>
<td>(shake flask, Hansch et al. 1973)</td>
<td>4.04</td>
</tr>
<tr>
<td>(Neely et al. 1974; Hansch &amp; Leo 1979)</td>
<td>4.17, 4.09, 3.16, 4.04</td>
</tr>
<tr>
<td>(HPLC-k′ correlation, Rekker &amp; De Kort 1979)</td>
<td>3.95</td>
</tr>
<tr>
<td>(HPLC-RT correlation, Veith et al. 1979a)</td>
<td>3.75</td>
</tr>
<tr>
<td>(shake flask-HPLC, Banerjee et al. 1980)</td>
<td>4.04</td>
</tr>
<tr>
<td>(lit. average, Kenaga &amp; Goring 1980; Freitag et al. 1985)</td>
<td>3.88</td>
</tr>
<tr>
<td>(RP-TLC-k′ correlation, Bruggeman et al. 1982)</td>
<td>4.10</td>
</tr>
<tr>
<td>(HPLC-k′ correlation, Hammers et al. 1982)</td>
<td>4.08</td>
</tr>
<tr>
<td>(HPLC-RT correlation, Woodburn 1982; Woodburn et al. 1984)</td>
<td>3.70</td>
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<tr>
<td>(shake flask, range, average, Eadsforth &amp; Moser, 1983)</td>
<td>3.16-4.09, 3.91</td>
</tr>
<tr>
<td>(HPLC, range, average, Eadsforth &amp; Moser 1983)</td>
<td>3.91-4.15, 4.05</td>
</tr>
<tr>
<td>(HPLC-k′ correlation, Hafkenscheid &amp; Tomlinson 1983)</td>
<td>4.03</td>
</tr>
<tr>
<td>(HPLC correlation; Harnisch et al. 1983)</td>
<td>3.93</td>
</tr>
<tr>
<td>(generator column-GC/ECD, Miller et al. 1984,1985)</td>
<td>3.76</td>
</tr>
<tr>
<td>(generator column-HPLC, Woodburn et al. 1984)</td>
<td>3.89</td>
</tr>
<tr>
<td>(RP-HPLC-RT correlation, Rapaport &amp; Eisenreich 1984)</td>
<td>3.79</td>
</tr>
<tr>
<td>(HPLC-RV correlation, quoted exp. Garst 1984)</td>
<td>4.11-4.13</td>
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<tr>
<td>(HPLC-RV correlation, Garst &amp; Wilson 1984)</td>
<td>4.10</td>
</tr>
<tr>
<td>(HPLC-RT correlation, Edsforth 1986)</td>
<td>4.05</td>
</tr>
<tr>
<td>(shake flask-GC, Menges &amp; Armstrong 1991)</td>
<td>3.81</td>
</tr>
<tr>
<td>(HPLC-RT correlation, Wang et al. 1986)</td>
<td>4.13</td>
</tr>
<tr>
<td>(HPLC-k′ correlation, De Kock &amp; Lord 1987)</td>
<td>3.63</td>
</tr>
<tr>
<td>(generator column-GC, Doucette &amp; Andren 1987, 1988)</td>
<td>3.89</td>
</tr>
<tr>
<td>(RP-HPLC-RI correlation, Brodsky &amp; Ballschmiter 1988)</td>
<td>4.14, 4.06, 4.00, 3.94</td>
</tr>
<tr>
<td>(HPLC-RT correlation, Doucette &amp; Andren 1988)</td>
<td>3.69</td>
</tr>
<tr>
<td>(HPLC-RT correlation, Sherblom &amp; Eganhouse 1988)</td>
<td>3.75</td>
</tr>
<tr>
<td>(slow stirring-GC; calculated-π const., De Bruijn et al. 1989; De Bruijn &amp; Hermens 1990)</td>
<td>4.008; 4.10</td>
</tr>
<tr>
<td>(recommended, Sangster 1989, 1993)</td>
<td>3.98</td>
</tr>
<tr>
<td>(dual-mode centrifugal partition chromatography, Gluck &amp; Martin 1990)</td>
<td>4.29</td>
</tr>
<tr>
<td>(HPLC-k′ correlation, Noegrohati &amp; Hammers 1992)</td>
<td>4.26</td>
</tr>
<tr>
<td>(recommended, Hansch et al. 1995)</td>
<td>4.01</td>
</tr>
</tbody>
</table>

Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 20°C, multi-column GC-k′ correlation; calculated at 20°C, Zhang et al. 1999)</td>
<td>6.92, 6.09; 6.09</td>
</tr>
<tr>
<td>(calculated-S∞, and vapor pressure P, Abraham et al. 2001)</td>
<td>6.15</td>
</tr>
</tbody>
</table>

Bioconcentration Factor, log BCF:

<table>
<thead>
<tr>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(trout, calculated-k1/k2, Neely et al. 1974)</td>
<td>2.64</td>
</tr>
<tr>
<td>(rainbow trout, Veith et al. 1979; Veith &amp; Kosian 1983)</td>
<td>3.12</td>
</tr>
<tr>
<td>(fish, flowing water, Kenaga &amp; Goring 1980; Kenaga 1980)</td>
<td>2.53</td>
</tr>
<tr>
<td>(algae, fish, activated sludge, Freitag et al. 1985; selected, Halfon &amp; Reggiani 1986)</td>
<td>2.73, 2.45, 3.41</td>
</tr>
</tbody>
</table>
Sorption Partition Coefficient, log $K_{OC}$:

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 mg/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 mg/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)
4.20; 3.30 (soil, calculated-universal solvation model; quoted lit., Winget et al. 2000)
3.03, 3.12 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, average values, Delle Site 2001)

Sorption Partition Coefficient, log $K_P$:

2.146 (lake sediment, calculated-$K_{OW}$ $f_{OC}$, Formica et al. 1988)

Environmental Fate Rate Constants, k and Half-Lives, $t_\text{½}$:

Volatile/Evaporation: $t_\text{½} = 7.52$ d evaporation from water depth of 1 m (Mackay & Leinonen 1975), rate of volatilization $k = 0.92$ g m$^{-2}$ h$^{-1}$ (Metcalfe et al. 1988)
Photolysis: $k = 5.1 \times 10^{-4}$ h$^{-1}$ to $7.4 \times 10^{-3}$ h$^{-1}$ with H$_2$O$_2$ under photolysis at 25°C in F-113 solution and with HO$^-$ in the gas (Dilling et al. 1988);
photodegradation $k = 5.1 \times 10^{-4}$ min$^{-1}$ and $t_\text{½} = 22.61$ h in methanol-water (3:7, v/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, $k_{OH}$ for reaction with OH radical, $k_{NO_3}$ with NO$_3$ radical and $k_{O_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:
$k_{OH} = (8.06 \pm 0.77) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with an estimated lifetime of ~3 d, and $k_{O_3} < 2.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 294 $\pm$ 1 K (relative rate method, Atkinson et al. 1984)
$k_{OH} = (8.5 \pm 0.8) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 295 K (relative rate method, Atkinson & Aschmann 1988)
$k_{OH} = (7 \pm 2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1985)
$k_{OH}^{(calc)} = 7.9 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(obs.)} = (5.8 \pm 8.2) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated tropospheric lifetime of 3 d (Atkinson 1987a)
$k_{OH}^{(calc)} = 7.1 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(obs.)} = 7.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (SAR structure-activity relationship, Atkinson 1987b)
$k_{SO_2} = 2 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{OH} = 7.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$; $k_{NO_3} < 2.0 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ for reaction with NO$_3$ at room temp. (Atkinson & Aschmann 1988)
$k_{OH}^{(calc)} = 7.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (recommended, Atkinson 1989)
$k_{OH}^{(calc)} = 6.64 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klant 1993)
$k_{OH}^{(exptl)} = 7.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}^{(calc)} = 6.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ 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);
$k = 10^9$ yr$^{-1}$ in the water column and $k = 1090$ yr$^{-1}$ in the sediment, microbial degradation pseudo first-order rate constant (Wong & Kaiser 1975; selected, Neely 1981);
$k = 9.3–9.8$ nmol L$^{-1}$ d$^{-1}$ with an initial biphenyl concentration of 4.4–4.7 $\mu$mol/L, and $k = 3.2$ nmol L$^{-1}$ d$^{-1}$ with initial concentration of 2.9 $\mu$mol/L, rate of biodegradation in water from Port Valdez (estimated, Reichardt et al. 1981)
$t_{½} = 1.5$ d, estimated by using water die-away test (Bailey et al. 1983)
$t_{½}^{(aq. aerobic)} = 36–168$ h, based on river die-away test data and activated sludge screening test data (Howard et al. 1991)
$t_{½}^{(aq. anaerobic)} = 144–672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
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removal rate of 5.3 and 0.52 mg (g of volatile suspended solid d)⁻¹, degradation by bacteria from creosote-
contaminated marine sediments with nitrate- and sulfate-reducers, respectively, under anaerobic condi-
tions in a fluidized bed reactor (Rockne & Strand 1998)

Biotransformation
Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:
k₁ = 6.79 h⁻¹; k₂ = 0.0155 h⁻¹ (trout muscle, Neely et al. 1974; Neely 1979)
k₁ = 6.8 h⁻¹; 1/k₂ = 65 h (trout, quoted, Hawker & Connell 1985)
log k₁ = 2.21 d⁻¹; log 1/k₂ = 0.43 d (fish, Connell & Hawker 1988)
log k₂ = −0.43 d⁻¹ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:
Air: calculated lifetime of ~3 d due to reaction with OH radical, assuming an average daytime atmospheric OH
radical concn of ~1 × 10⁶ molecule/cm³ (Atkinson et al. 1984);
estimated atmospheric lifetime of ~2.7 d due to reaction with the OH radical for a 24-h average OH radical
concn of 5 × 10⁶ 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);
tₜₒ = 7.8–110 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: tₜₒ ~1.5 d in river water (Bailey et al. 1983);
tₜₒ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
photolysis tₜₒ = 19.18 min in aqueous solution when irradiated with a 500 W medium pressure mercury
lamp (Chen et al. 1996).
Groundwater: tₜₒ = 72–336 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Sediment:
Soil: tₜₒ = 36–168 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)
Biota: estimated tₜₒ = 29 h from fish in simulated ecosystem (Neely 1980).

**TABLE 4.1.13.1**
Reported aqueous solubilities of biphenyl at various temperatures

<table>
<thead>
<tr>
<th>Bohon &amp; Claussen 1951</th>
<th>Wauchope &amp; Getzen 1972</th>
<th>Shaw 1989</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>t/°C</strong></td>
</tr>
<tr>
<td><strong>shake flask-UV</strong></td>
<td><strong>shake flask-UV</strong></td>
<td></td>
</tr>
<tr>
<td>0.40</td>
<td>2.83</td>
<td>24.6</td>
</tr>
<tr>
<td>2.4</td>
<td>2.97</td>
<td>24.6</td>
</tr>
<tr>
<td>5.2</td>
<td>3.38</td>
<td>24.6</td>
</tr>
<tr>
<td>7.6</td>
<td>3.64</td>
<td>29.9</td>
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<td>10</td>
<td>4.06</td>
<td>29.9</td>
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<tr>
<td>12.6</td>
<td>4.58</td>
<td>29.9</td>
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<td>14.9</td>
<td>5.11</td>
<td>30.3</td>
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<td>15.9</td>
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<td>30.3</td>
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<tr>
<td>25</td>
<td>7.48</td>
<td>30.3</td>
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<tr>
<td>25.6</td>
<td>7.78</td>
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<td>30.1</td>
<td>9.64</td>
<td>38.4</td>
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<tr>
<td>30.4</td>
<td>9.58</td>
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<td>33.3</td>
<td>11.0</td>
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<td>34.9</td>
<td>11.9</td>
<td>40.1</td>
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<td>36</td>
<td>12.5</td>
<td>40.1</td>
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<td>42.8</td>
<td>17.2</td>
<td>47.5</td>
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</table>

(Continued)
TABLE 4.1.13.1 (Continued)

<table>
<thead>
<tr>
<th>Bohon &amp; Claussen 1951</th>
<th>Wauchope &amp; Getzen 1972</th>
<th>Shaw 1989</th>
<th>IUPAC recommended</th>
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</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>for supercooled liquid:</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>ΔH_mol/(kJ mol⁻¹) =</td>
<td></td>
<td></td>
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<tr>
<td>at 275 K</td>
<td>7.03</td>
<td>50.1</td>
<td>20.6</td>
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<tr>
<td>280 K</td>
<td>10.13</td>
<td>50.1</td>
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<td>285 K</td>
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<td></td>
<td>64.5</td>
<td>46.5</td>
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</tbody>
</table>

Empirical temperature dependence equations:

Wauchope & Getzen (1972): 

\[ R \cdot \ln x = -\frac{\Delta H_{\text{mol}}}{(T/K)} + (0.000408)[(T/K) - 291.15]^2 - c + b(T/K) \]  

(1)

![Biphenyl: solubility vs. 1/T](image)

FIGURE 4.1.13.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for biphenyl.
TABLE 4.1.13.2
Reported vapor pressures of biphenyl at various temperatures and the coefficients for the vapor pressure equations

\[
\log P = A - B/(T/K) \quad (1)
\]

\[
\ln P = A - B/(T/K) \quad (1a)
\]

\[
\log P = A - B/(C + t/°C) \quad (2)
\]

\[
\ln P = A - B/(C + t/°C) \quad (2a)
\]

\[
\log P = A - B/(C + T/K) \quad (3)
\]

\[
\log P = A - B/(T/K) - C \cdot \log(T/K) \quad (4)
\]

\[
\log P = A - B/(T/K) - C \cdot \log(T/K)^2 \quad (5)
\]

1.

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<tr>
<th>Chipman &amp; Peltier 1929</th>
<th>Stull 1947</th>
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<th>Bradley &amp; Cleasby 1953</th>
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bp/°C 266.25
\[\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 72.80\]
at bp

eq. 5 P/mmHg
A 7.0220
B 1723
C 245700
temp range 162–322°C

2.

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(Continued)
### TABLE 4.1.13.2 (Continued)

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<td>B 4367.436</td>
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<td>for temp range 24.9–50°C</td>
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|                       | Sharma & Palmer 1974 |
|                       | gas saturation-GC    |
| t/°C                  | P/Pa |
| 53.05                 | 16.0 |
| 61.05                 | 34.66|
| 71.95                 | 92.0 |
| 81.05                 | 220.0|

**FIGURE 4.1.13.2** Logarithm of vapor pressure versus reciprocal temperature for biphenyl.
4.1.1.14 4-Methylbiphenyl

Chemical Structure:

Common Name: 4-Methylbiphenyl
Synonym: 4-phenyltoluene
Chemical Name: 4-methylbiphenyl
CAS Registry No: 644-08-6
Molecular Formula: C_{13}H_{12}
Molecular Weight: 168.234
Melting Point (°C):
- 49.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
- 165.7 (27°C, calculated-density)
- 206.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Evaporation, ΔH_{vap} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.575 (mp at 49.5°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations.):
- 1.834, 4.05, 7.03 (4.9, 25, 40°C, generator column-HPLC/GC, Doucette & Andren 1988a)
- S/(mol/L) = 9.18 × 10⁻⁶ exp(0.038·t/°C) (generator column-GC/ECD, temp range 4.9–40°C, Doucette & Andren 1988a); or
- log x = –1436/(T/K) – 1.541; temp. range 4.9–40°C (generator column-GC/ECD, Doucette & Andren 1988a)

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{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 K_{oa}:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k or Half-Lives, 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: C₁₄H₁₄
Molecular Weight: 182.261
Melting Point (°C):
125 (Weast 1982–83; Ruelle & Kesselring 1997; Lide 2003)
Boiling Point (°C):
295 (Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
194.0 (Ruelle & Kesselring 1997)
229.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Evaporation, ΔH_v (kJ/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 0.104 (mp at 125°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations.):
0.0687, 0.175, 0.441 (4.9, 25, 40°C, generator column-GC, Doucette & Andren 1988a)
S/(mol/L) = 2.90 × 10⁻⁷ exp(0.052·t°C) (generator column-GC/ECD, temp range 4–40°C, Doucette & Andren 1988a)
\[ \log x = -1913/(T/K) - 1.288; \text{ temp. range } 4.9–40°C \] (generator column-GC/ECD, Doucette & Andren 1988a)
Vapor Pressure (Pa at 25°C):
0.931 (calculated-P/C)
Henry’s Law Constant (Pa m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{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 K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oe}:
Environmental Fate Rate Constants, k or Half-Lives, t₁/₂:
Half-Lives in the Environment:
4.1.1.16 Diphenylmethane

Common Name: Diphenylmethane
Synonym: diphenyl methane, 1,1′-methylenebis-benzene
Chemical Name: diphenylmethane
CAS Registry No: 101-81-5
Molecular Formula: C\textsubscript{13}H\textsubscript{12}
Molecular Weight: 168.234
Melting Point (°C):
\begin{itemize}
  \item 25.4 \quad (Lide 2003)
\end{itemize}
Boiling Point (°C):
\begin{itemize}
  \item 265 \quad (Lide 2003)
\end{itemize}
Density (g/cm\textsuperscript{3} at 20°C):
\begin{itemize}
  \item 1.00592, 1.00192 \quad (20°C, 25°C. Dreisbach 1955)
  \item 1.001 \quad (26°C Lide 2003)
\end{itemize}
Molar Volume (cm\textsuperscript{3}/mol):
\begin{itemize}
  \item 168.1 \quad (27°C, from density, Stephenson & Malanowski 1987)
  \item 167.2 \quad (20°C, calculated-density)
  \item 206.8 \quad (calculated-Le Bas method at normal boiling point)
\end{itemize}
Enthalpy of Evaporation, \(\Delta H_v\) (kJ/mol):
\begin{itemize}
  \item 64.02 \quad (Bright 1951)
  \item 66.845, 45.34 \quad (25°C, bp, Dreisbach 1955)
\end{itemize}
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
\begin{itemize}
  \item 18.28 \quad (Dreisbach 1955)
  \item 18.58 \quad (Parks & Huffman 1931; Chickos et al. 1999)
\end{itemize}
Entropy of Fusion, \(\Delta S_{ fus}\) (J/mol K):
\begin{itemize}
  \item 61.92 \quad (Stephenson & Malanowski 1987)
  \item 62.34, 62.1 \quad (exptl., calculated-group additivity method, Chickos et al. 1999)
\end{itemize}
Fugacity Ratio at 25°C (assuming \(\Delta S_{ fus} = 56\) J/mol K), F: 0.991 (mp at 25.4°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
\begin{itemize}
  \item 14.10 \quad (shake flask/UV, Andrews and Keefer 1949)
  \item 16.40 \quad (Deno & Berkheimer 1960)
  \item 3.76 \quad (Lu et al. 1978)
  \item 3.00 \quad (shake flask-nephelometry, Hollifield 1979)
  \item 16.19 \quad (lit. mean, Pearlman et al. 1984)
\end{itemize}

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):
\begin{itemize}
  \item 133.3* \quad (76.0°C, summary of literature data, temp range 76.0–264.5°C, Stull 1947)
  \item 1.09 \quad (effusion method, interpolated from reported Antoine eq., Bright 1951)
\end{itemize}
\begin{align*}
\log (P:mmHg) &= 9.12 – 3341/(T/K); \text{ temp range } 5.1–26.5°C \quad \text{(Antoine eq., effusion, Bright 1951)} \\
2.266 &= \text{(calculated by formula, Dreisbach 1955)} \\
\log (P:mmHg) &= 7.16125 – 1944.42/(190.0 + t/°C); \text{ temp range } 150–310°C \quad \text{(Antoine eq. for liquid state, Dreisbach 1955)} \\
3904* &= \text{(151.49°C, static-differential pressure gauge, measured range 151.49–336.32°C, Wieczorek & Kobayashi 1980)} \\
0.0452 &= \text{(extrapolated-Antoine eq., Boublik et al. 1984)} \\
\log (P:kPa) &= 5.94201 – 1668.355/(186.212 + t/°C); \text{ temp range } 217.5–282.2°C \quad \text{(Antoine eq. from reported exptl. data, Boublik et al. 1984)}
\end{align*}
Reported vapor pressures of diphenylmethane at various temperatures and the coefficients for the vapor pressure equations

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<thead>
<tr>
<th>Summary of literature data</th>
<th>Bright 1951</th>
<th>Wieczorek &amp; Kobayashi 1980</th>
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#### Klara et al. 1987

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fitted to Chebyshev Polynomial

$\Delta H_{vap} (kJ \cdot mol^{-1}) = 88.48$ at 284.3 K

$\Delta H_{vap} (kJ \cdot mol^{-1}) = 87.63$ at 298.15 K

**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: C\textsubscript{14}H\textsubscript{14}
Molecular Weight: 182.261
Melting Point (°C):
52.5 (Lide 2003)
Boiling Point (°C):
284 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.9780 (25°C Lide 2003)
Molar Volume (cm\textsuperscript{3}/mol):
190.2 (60°C, calculated-density, Stephenson & Malanowski 1987)
186.4 (25°C, calculated-density)
229.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
23.43 (Parks & Huffman 1931)
30.54 (Stephenson & Malanowski 1987)
22.73 (Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
94.14 (Stephenson & Malanowski 1987)
Fugacity Ratio at 25°C (assuming $\Delta S = 56$ J/mol K), F: 0.537 (mp at 52.5°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°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°C and reported temperature dependence equations. Additional data at other temperatures designated ∗, are compiled at the end of this section):
133.3* (86.8°C, summary of literature data, temp range 86.8–284.0°C, Stull 1947)
0.198 (effusion method, interpolated from reported Antoine eq., Bright 1951)
log (P/mmHg) = 9.86 – 3783/(T/K); temp range 17.1–44.2°C (Antoine eq., effusion, Bright 1951)
17.1* (60°C, inclined piston, measured range 60–140°C, Osborn & Scott 1980)
log (P/atm) = [1– 547.288/(T/K)] × 10\textsuperscript{0.914704 – 6.08831 × 10\textsuperscript{-4}·(T/K) + 5.11258 × 10\textsuperscript{-7}·(T/K)\textsuperscript{2}}; temp range 333.15–413.15 K, (Cox eq., Chao et al. 1983)
0.406 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P\textsubscript{L}/kPa) = 11.319 – 4386/(T/K), temp range 286–308 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
log (P\textsubscript{L}/kPa) = 6.93271 – 2636.21/(-22.009 + T/K); temp range 369–557 K (Antoine eq.-II, Stephenson & Malanowski 1987)
log (P/mmHg) = 48.5573 – 5.2841 × 10\textsuperscript{-3}·(T/K) – 13.41·log (T/K) – 1.0073 × 10\textsuperscript{-9}·(T/K) + 2.1338 × 10\textsuperscript{-6}·(T/K)\textsuperscript{2}; temp range 324–780 K (vapor pressure eq., Yaws 1994)
0.734; 0.249 (supercooled liquid $P\textsubscript{L}$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)
log (P\textsubscript{L}/Pa) = -3522/(T/K) + 11.67; $\Delta H_{\text{vap}} = -67.4$ kJ·mol\textsuperscript{-1} (GC-RT correlation, Lei et al. 2002)

Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Water Partition Coefficient, log $K_{OW}$:
- 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 ± 0.20 (recommended, Sangster 1989)
- 4.79 (recommended, Sangster 1993)
- 4.79 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_\frac{1}{2}$:

Half-Lives in the Environment:

**TABLE 4.1.17.1**
Reported vapor pressures of bibenzyl at various temperatures and the coefficients for the vapor pressure equations

| T/°C | P/Pa  | | T/°C | P/Pa  | | T/°C | P/Pa  |
|------|-------| |      |       | |      |       |
| 86.8 | 133.3 | | 60   | 17.1  |
| 119.8| 666.6 | | 65   | 24.1  |
| 136.0| 1333  | | 70   | 34.0  |
| 153.7| 2666  | | eq. 1| P/mmHg|
| 173.7| 5333  | | A    | 9.56  |
| 186.0| 7999  | | B    | 3783  |
| 202.8| 13332 | | temp range 17.1–44.2°C | |
| 227.8| 26664 | | 90   | 121.2 |
| 255.0| 53329 | | \(\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 72.38\) | |
| 284.0| 101325| | 100  | 213.6 |
| mp/°C| 51.5  | | 105  | 280.1 |
|       |       | | 110  | 364.2 |

| T/°C | P/Pa  | | T/°C | P/Pa  |
|------|-------| |      |       |
| 115  | 469.8 |
| 120  | 602.4 |
| 125  | 761.8 |
| 130  | 961.1 |
| 135  | 1202.7|
| 140  | 1498  |

Data fitted to a 4–constant vapor pressure eq.
FIGURE 4.1.17.1 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: C\textsubscript{14}H\textsubscript{12}
Molecular Weight: 180.245
Melting Point (°C):
124.2 (Lide 2003)
Boiling Point (°C):
307 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
0.9707 (Weast 1982–83; Lide 2003)
Molar Volume (cm\textsuperscript{3}/mol):
185.0 (Ruelle & Kesselring 1997)
185.7 (20°C, calculated-density)
221.6 (calculated-Le Bas method at normal boiling point)
Enthalpy of Sublimation, Δ\textsubscript{H\textsubscript{subl}} (kJ/mol):
100.7 (Van Ekeren et al. 1983)
Enthalpy of Fusion, Δ\textsubscript{H\textsubscript{fus}} (kJ/mol):
30.125 (Stephenson & Malanowski 1987)
27.40 (Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, Δ\textsubscript{S\textsubscript{fus}} (J/mol K):
76.73 (Stephenson & Malanowski 1987)
68.81, 69.7 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming Δ\textsubscript{S\textsubscript{fus}} = 56 J/mol K), F: 0.106 (mp at 124.2°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
0.29 (shake flask-UV, Andrews & Keefer 1950)
Vapor Pressure (Pa at 25°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* (113.2°C, summary of literature data, temp range 113.2–306.5°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 (34.65°C, effusion-quartz crystal microbalance, Offringa et al. 1983)
0.00647 (interpolated-Antoine eq., Stephenson & Malanowski 1987)
log (P\textsubscript{s}/kPa) = 12.25604 – 5201.358/(T/K); temp range 298–343 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
log (P\textsubscript{s}/kPa) = 6.97928 – 2610.05/(-54.759 + T/K); temp range 419–580 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
log (P/mmHg) = 68.6303 – 6.3776 × 10\textsuperscript{3}/(T/K) – 21.015·log (T/K) + 5.7813 × 10\textsuperscript{-3}·(T/K)\textsuperscript{2}; temp range 397–820 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C):
Octanol/Water Partition Coefficient, log K\textsubscript{OW}:
4.81 (Hansch & Leo 1979)
4.81 (recommended, Sangster 1989)
4.81 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log $K_{OA}$:
7.48 (calculated-$S_{oc}$ and vapor pressure $P$, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 4.1.1.18.1</th>
<th>Reported vapor pressures of trans-stilbene at various temperatures and the coefficients for the vapor pressure equations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>log $P = A - B/(T/K)$</td>
</tr>
<tr>
<td></td>
<td>log $P = A - B/(C + t/°C)$</td>
</tr>
<tr>
<td></td>
<td>log $P = A - B/(C + T/K)$</td>
</tr>
<tr>
<td></td>
<td>log $P = A - B/(T/K) - C\cdot\log (T/K)$</td>
</tr>
<tr>
<td></td>
<td>$\Delta H_{fus} = 100.17 \text{ kJ/mol}$ at 331.64 K</td>
</tr>
</tbody>
</table>

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FIGURE 4.1.18.1 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: C₁₂H₈
Molecular Weight: 152.192
Melting Point (°C):
91.8 (Lide 2003)
Boiling Point (°C):
280 (Lide 2003)
Density (g/cm³ at 20°C):
0.899 (Dean 1985)
0.8987 (17°C, Lide 2003)
Molar Volume (cm³/mol):
141.2 (Ruelle & Kesselring 1997)
167.1 (17°C, calculated-density)
165.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
10.96 (Ruelle & Kesselring 1997)
1.4, 6.95, 10.96; 12.36 (~156.55, 88.45, 88.85°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol 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°C (assuming ΔS_{fus} = 56 J/mol K), F:
0.221 (mp at 91.8°C)
0.458 (calculated, ΔS_{fus} = 30.3 J/mol K, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C and reported temperature dependence equations):
3.93 (misquoted from Mackay & Shiu 1977)
16.1 (generator column-HPLC/fluorescence, Walters & Luthy 1984)
log [Sₗ/(mol/L)] = 1.315 – 573.5/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°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/fluor./UV, Sonnefeld et al. 1983)
log (P/Pa) = 12.768 – 3821.55/(T/K); temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)
0.893 (generator column-HPLC, Waski et al. 1983)
1.105 (interpolated, Antoine eq., Stephenson & Malanowski 1987)
log (Pₗ/kPa) = 9.500 – 3714/(T/K); temp range 286–318 K (Antoine eq., Stephenson & Malanowski 1987)
0.90 (selected, Mackay et al. 1992, 1996; quoted, Shiu & Mackay 1997)
0.90; 1.97 (quoted solid Pₗ from Mackay et al. 1992; converted to supercooled liquid Pₗ with fugacity ratio F; Passivirta et al. 1999)
log (Pₗ/Pa) = 11.11 – 3201/(T/K) (solid, Passivirta et al. 1999)
log (Pₗ/Pa) = 9.53 – 2751/(T/K) (supercooled liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa m³/mol at 25°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°C, Bamford et al. 1999)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

\[ \ln K_{NW} = -6278.6/(T/K) + 15.757; \Delta H = 52.2 \text{ kJ mol}^{-1}; \text{measured range} 4.1-31^\circ \text{C (gas stripping-GC, Bamford et al. 1999)} \]

\[ \log \left[ H/(Pa \text{ m}^3/\text{mol}) \right] = 8.22 - 2178/(T/K) \] (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):
- 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 \( \gamma \) 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, \( \log K_{OA} \):

Bioconcentration Factor, \( \log BCF \):
- 3.0 (microorganisms-water, calculated-\( K_{OW} \), Mabey et al. 1982)
- 2.58 (Isnard & Lambert 1988)

Sorption Partition Coefficient, \( \log K_{OC} \) at 25°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)
- 4.96; 5.05, 5.14, 5.45 (20°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, \( t_{1/2} \):

Volatilization:
- Photolysis: not environmentally significant (Mabey et al. 1982);
  - \( t_{1/2} = 0.7 \text{ h on silica gel, } t_{1/2} = 2.2 \text{ h on alumina and } t_{1/2} = 44 \text{ h on fly ash for different atmospheric particulate substrates determined in the rotary photoreactor (appr. 25 \mu \text{g/g on substrate) (Behymer & Hites 1985); direct photolysis } t_{1/2} = 9.08 \text{ h (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).}}
- Photodegradation \( k = 3 \times 10^{-3} \text{ s}^{-1} \) in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)
- Oxidation: rate constant \( k \) for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO\(_3\) radical and \( k_{O_3} \) with O\(_3\) or as indicated, *data at other temperatures see reference:
  - \( k = 4 \times 10^{7} \text{ M}^{-1} \text{ h}^{-1} \) for singlet oxygen and \( k = 5 \times 10^{7} \text{ M}^{-1} \text{ h}^{-1} \) for peroxy radical (calculated, Mabey et al. 1982)
  - \( k_{OH} = 5.50 \times 10^{-16} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1}, k_{OH} = (11.0 \pm 0.1) \times 10^{-11} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} \) and \( k_{NO_3} = (54 \pm 0.8) \times 10^{-12} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} \) at 296 ± 2 K (relative rate methods, Atkinson & Aschmann 1988)
  - \( k_{OH} = 11.0 \times 10^{-11} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} \) at 296 K (Atkinson 1989)
  - \( k_{OH} = 12.4 \times 10^{-11} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} \) at 296 ± 2 K with a atmospheric lifetime of 1.1 h assuming an average ambient 12-h daytime OH radical concn of \( 2 \times 10^6 \text{ molecule/cm}^3 \); \( k_{O_3} = 1.60 \times 10^{-16} \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} \) at 296 K with lifetime of 2.5 h assuming ambient O\(_3\) concn of 7 × 10\(^{11}\) molecule/cm\(^3\) (relative rate method, Reisen & Arey 2002)
- Biodegradation: > 98% degradation within 7 d, based on domestic sewer for an average of three static-flask screening test (Tabak et al. 1981); aerobic \( t_{1/2} = 1020-1440 \text{ h, based on soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991)} \);
  - anaerobic \( t_{1/2} = 4080-5760 \text{ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).}}
- Biotransformation: \( k = 3 \times 10^{-9} \text{ mL cell}^{-1}\text{h}^{-1} \), estimated rate constant for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:
Half-Lives in the Environment:
Air: $t_{1/2} = 0.191–1.27$ 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 O$_3$ at 296 K, respectively (Reisens & Arey 2002)
Surface water: $t_{1/2} = 1020–1440$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Kincannon & Lin 1985; quoted, Howard et al. 1991).
Groundwater: $t_{1/2} = 2040–2880$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Sediment:
Soil: $t_{1/2} = 1020–1440$ h, based on soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991);
$t_{1/2} > 50$ d (Ryan et al. 1988).
Biota: elimination $t_{1/2} = 1$ d from rainbow trout (quoted, Meador et al. 1995).

### TABLE 4.1.1.19.1
Reported vapor pressures and Henry's law constants of acenaphthylene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Vapor pressure</th>
<th>Henry's law constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>gas saturation-HPLC</td>
</tr>
<tr>
<td>$t/^{°C}$</td>
<td>P/Pa</td>
</tr>
<tr>
<td>11.20</td>
<td>0.206</td>
</tr>
<tr>
<td>11.20</td>
<td>0.205</td>
</tr>
<tr>
<td>11.20</td>
<td>0.216</td>
</tr>
<tr>
<td>20.56</td>
<td>0.590</td>
</tr>
<tr>
<td>20.56</td>
<td>0.585</td>
</tr>
<tr>
<td>30.40</td>
<td>1.50</td>
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<td>30.40</td>
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<td>30.40</td>
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<tr>
<td>39.05</td>
<td>3.41</td>
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<tr>
<td>39.05</td>
<td>3.27</td>
</tr>
<tr>
<td>39.05</td>
<td>3.34</td>
</tr>
<tr>
<td>25.0</td>
<td>0.89</td>
</tr>
</tbody>
</table>

$log P/Pa = A - B/(T/\text{K})$

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: C_{12}H_{10}
Molecular Weight: 154.207
Melting Point (°C):
93.4 (Lide 2003)
Boiling Point (°C):
279 (Weast 1982–82; Lide 2003)
Density (g/cm³ at 20°C):
1.069 (95°C, Dean 1985)
1.222 (Lide 2003)
Molar Volume (cm³/mol):
126.2 (20°C, calculated-density)
173.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
84.68 (Radchenko & Kitiagorodskii 1974)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
21.88 (differential calorimetry, Wauchope & Getzen 1972)
21.46 (calorimetry, Osborn & Douslin 1975; Chickos et al. 1999)
Entropy of Fusion, ΔS_{ fus} (J/mol 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°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.213 (mp at 93.4°C)
0.197 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°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°C, Wauchope & Getzen 1972)
R ln x = −5230/(T/K) + 4.08 × 10⁻⁴ [(T/K) − 291.15]² − 17.1 + 0.0186(T/K); temp range 22.2–73.4°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 [S_L/(mol/L)] = 2.505 − 1127/(T/K) (supercooled liquid S_L, Passivirta et al. 1999)
ln x = 0.684974 − 4541.77/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2560* (147.2°C, static isoteniscope method, measured range 147.2–287.8°C, Mortimer & Murphy 1923)
\[ \log (P/\text{mmHg}) = 8.033 - 2835/(T/K); \text{ temp range } 147.2–287.8°C \]

666.6* (114.8°C, summary of literature data, temp range 114.8–277.5°C, Stull 1947)
\[ \log (P/\text{mmHg}) = 11.50 - 4264/(T/K); \text{ temp range } –15 \text{ to } 30°C \]

66.6* (114.8°C, summary of literature data, temp range 114.8–277.5°C, Stull 1947)
\[ \log (P/\text{mmHg}) = 11.50 - 4264/(T/K); \text{ temp range } –15 \text{ to } 30°C \]

4.02 (extrapolated-Antoine eq., Hoyer & Peperle 1958)
\[ \log (P/\text{mmHg}) = 0.207 \]
\[ \log (P/\text{mmHg}) = 11.50 - 4264/(T/K); \text{ temp range } –15 \text{ to } 30°C \]

8.622* (54.1°C, effusion method, measured range 54.1–83.45°C, Radchenko & Kitiagorodskii 1974)
\[ \log (P/\text{mmHg}) = 12.2930 - 4422.921/(T/K); \text{ temp range } 54.10–83.15°C \]

0.373* (manometry-extrapolated, measured range 65–140°C, Osborn & Douslin 1975)
\[ \log (P/\text{Pa}) = 22.9288 - 5183.86/(T/K – 80.153); \text{ temp range: } 293.1–342 \text{ K} \]

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

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, Fendiger & 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°C, Bamford et al. 1999)

\[ \ln K_{AW} = -6242.48/(T/K) + 16.0, \Delta H = 51.9 \text{ kJ mol}^{-1}; \text{ measured range 4.1–31°C, (gas stripping-GC, Bamford et al. 1999)} \]

\[ \log \left( \frac{H}{(\text{Pa m}^3/\text{mol})} \right) = 5.63 - \frac{1240}{(T/K)} \] (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log \( K_{OW} \) at 25°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 (23°C, shake flask, Banerjee et al. 1980)
3.92 (recommended, Sangster 1989, 1993)
3.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log \( K_{OA} \) at 25°C:

6.31 (calculated-Soct and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log \( BCF \):

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 \( K_{OC} \) at 25°C or as indicated:

5.38 (sediments average, Kayal & Connell 1990)
3.79 (RP-HPLC correlation on CIHAC, Szabo 1999b)
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 (20°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, \( t_{1/2} \):

Volatilization:

Photolysis: half-lives on different atmospheric substrates determined in the rotary photoreactor (appr. 25 µg/g on substrate): \( t_{1/2} = 2.0 \text{ h on silica gel, } t_{1/2} = 2.2 \text{ h on alumina and } t_{1/2} = 44 \text{ h on fly ash (Behymer & Hites 1985); } \)
\( k = 0.23 \text{ h}^{-1} \) in distilled water with \( t_{1/2} = 3 \text{ h (Fukuda et al. 1988); } \)
\( \text{direct photolysis } t_{1/2} = 7.67 \text{ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).} \)

Hydrolysis: not hydrolyzable (Mabey et al. 1982).

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{OH} \) for reaction with OH radical, \( k_{NO_3} \) with NO \(_3\) radical and \( k_{O_3} \) with O \(_3\) as or indicated, *data at other temperatures see reference:

\( k < 3600 \text{ M}^{-1} \text{ h}^{-1} \) for singlet O \(_2\), \( k = 8000 \text{ M}^{-1} \text{ h}^{-1} \) for peroxo radical at 25°C (Mabey et al. 1982)
\( k_{OH}(\text{exptl}) = 1.03 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH}(\text{calc}) = 1.49 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) (Atkinson et al. 1988)
\( k_{O_3} < 5.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}, k_{OH} = (1.03 \pm 0.13) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) and \( k_{NO_3} = (4.6 \pm 2.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 ± 2 K (relative rate methods, Atkinson & Aschmann 1988)
\( k_{OH} = (103 – 58.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296–300 K (Atkinson 1989)
\( k_{OH}(\text{calc}) = 84.03 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) (molecular orbital calculations, Klamt 1996)
\( k_{OH}^* = 58 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 298 K, measured range 325–365 K with a calculated atmospheric lifetime of 4.9 h based on gas-phase OH reaction (Brubaker & Hites 1998)
\( k_{OH} = 8.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \) at 296 ± 2 K with an atmospheric lifetime of 1.8 h assuming an average ambient 12-h daytime OH radical concn of 2 × 10 \(^6\) molecule/cm\(^3\) (Reisen & Arey 2002)

Biodegradation: significant degradation within 7 d for a domestic sewer test (Tabak et al. 1981); aerobic \( t_{1/2} = 295–2448 \text{ h, based on aerobic soil column test data (Kincannon & Lin 1985; quoted, Howard et al. 1991);} \)
anaerobic $t_{1/2} = 1180$–$9792$ h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $3 \times 10^{-9}$ mL cell$^{-1}$ h$^{-1}$, estimated bacterial transformation rate constant (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Sorption ($k_1$)-Desorption ($k_2$) Rate constants: desorption rate constant of $0.018$ d$^{-1}$ with $t_{1/2} = 38.5$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:

Air: $t_{1/2} = 0.879$–$8.79$ 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: $t_{1/2} = 3$–$300$ h, based on photolysis half-life in water (Howard et al. 1991).

Groundwater: $t_{1/2} = 590$–$4896$ h, based on estimated unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption $t_{1/2} = 38.5$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 295$–$2448$ h, based on aerobic soil column test data (Kincannon & Lin 1985; quoted, Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: $t_{1/2} < 1.0$ 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

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Wauchope &amp; Getzen 1972</th>
<th>Shaw 1989</th>
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<td>$c$</td>
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TABLE 4.1.1.20.1 (Continued)

<table>
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<tr>
<th>t/°C</th>
<th>S/g·m⁻³</th>
<th>t/°C</th>
<th>S/g·m⁻³</th>
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<td>74.7</td>
<td>40.8</td>
<td>74.7</td>
<td>39.3</td>
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</table>

$\Delta H_{fus}/(kJ \cdot mol^{-1}) = 21.88$

Empirical temperature dependence equations:
Wauchope & Getzen (1972): $R \cdot \ln x = -\left[\frac{H_{fus}}{(T/K)}\right] + (0.000408)((T/K) - 291.15)^2 - c + b(T/K) \quad (1)$

FIGURE 4.1.1.20.1 Logarithm of mole fraction solubility ($\ln x$) 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

\[
\begin{align*}
\text{log } P &= A - B/(T/K) \quad (1) \\
\text{log } P &= A - B/(C + t/°C) \quad (2) \\
\text{log } P &= A - B/(C + T/K) \quad (3) \\
\text{log } P &= A - B/(T/K) - C \cdot \text{log } (T/K) \quad (4)
\end{align*}
\]

1. Mortimer & Murphy 1923  
   **static isotenoscope method**  
   **summary of literature data**  
   **effusion**  
   **effusion method**

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<th>t/°C</th>
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<th>t/°C</th>
<th>P/Pa</th>
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</table>

2. Osborn & Douslin 1975  
   **inclined-piston manometry**  
   Sonnefeld et al. 1983  
   **gas saturation-HPLC**  
   Sato et al. 1986  
   **gas saturation-electrobalance**

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<th>t/°C</th>
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<th>t/°C</th>
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**FIGURE 4.1.1.20.2** Logarithm of vapor pressure versus reciprocal temperature for acenaphthene.

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### TABLE 4.1.1.20.3
Reported Henry's law constants of acenaphthene at various temperatures

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<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>H/(Pa m³/mol)</th>
<th>average</th>
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</thead>
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<td>4.1</td>
<td>3.27, 3.79</td>
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<td>11.0</td>
<td>5.98, 6.62</td>
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<td>18.0</td>
<td>10.5, 11.4</td>
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<td></td>
</tr>
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<td>25.0</td>
<td>17.5, 19.6</td>
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<tr>
<td>31.0</td>
<td>26.5, 30.8</td>
<td>28.6</td>
<td></td>
</tr>
</tbody>
</table>

\[ \ln K_{AW} = A - B/(T/K) \]

- \( K_{AW} \)
- \( A = 15.997 \)
- \( B = 6242.5 \)

enthalpy, entropy change:
- \( \Delta H/(kJ \cdot mol^{-1}) = 51.9 \pm 1.3 \)
- \( \Delta S/(J \cdot K^{-1} \cdot mol^{-1}) = 133 \)

at 25°C

---

**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: C_{13}H_{10}
Molecular Weight: 166.218
Melting Point (°C): 114.77 (Lide 2003)
Boiling Point (°C): 295 (Dean 1985; Lide 2003)
Density (g/cm³ at 20°C): 1.203 (0°C, Lide 2003)
Molar Volume (cm³/mol):
138.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)
187.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{fu} \) (kJ/mol):
19.54 (Wauchope & Getzen 1972)
19.58 (Osborn & Douslin 1975; Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{fu} \) (J/mol 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°C (assuming \( \Delta S_{fu} = 56 \text{ J/mol K} \), F: 0.132 (mp at 114.77°C)
0.161 (calculated, \( \Delta S_{fu} = 50.5 \text{ J/mol K} \), Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°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°C, Wauchope & Getzen 1972)
\[ R \ln x = -4670/(T/K) + 4.08 \times 10^{-4}[(T/K) - 291.15]^2 - 24.2 + 0.0309(T/K); \text{ temp range 24.6–73.4°C (shake flask-UV measurements, Wauchope \\& Getzen 1972)} \]
1.98 (shake flask-fluorescence, Mackay & Shiu 1977)
1.68* (generator column-HPLC, measured range 6.6–31°C, May et al. 1978)
\[ S/(\mu g/kg) = 324.0 + 5.413(t/°C) + 0.8059(t/°C)^2 + 0.0025(t/°C)^3; \text{ temp range 4–29°C (generator column-HPLC/UV, May et al. 1978)} \]
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)
\[ \log [S_s/(mol/L)] = 1.664 - 1024/(T/K) \text{ (supercooled liquid, Passivirta et al. 1999)} \]
\[ \ln x = 0.82861 - 4824/(T/K); \text{ temp range 5–50°C (regression eq. of literature data, Shiu \\& Ma 2000)} \]
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2400* (161.0°C, static isoteniscope method, measured range 161.0–300.4°C, Mortimer & Murphy 1923)

\[ \log (P/\text{mmHg}) = 8.059 - 2957/(T/\text{K}) ; \text{ temp range 161–300.4°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)} \]

666.6* (129.3°C, summary of literature data, temp range 129.3–295.0°C, Stull 1947)

0.087* (effusion method, measured range 33.4–49.55°C, Bradley & Cleasby 1953)

\[ \log (P/\text{cmHg}) = 10.325 - 4324/(T/\text{K}) ; \text{ temp range 33.3–49.55°C (Antoine eq., Bradley & Cleasby 1953)} \]

1.66 (extrapolated-Antoine eq., liquid state \( P_L \), Weast 1972-73)

\[ \log (P/\text{mmHg}) = -0.2185 \times 13682.8/(T/\text{K}) + 8.18894 ; \text{ temp range 129.3–295°C (Antoine eq., Weast 1972–73)} \]

0.127* (static method-manometry, measured range 75.8–114°C, Osborn & Douslin 1975)

0.946 (Irwin 1982)

0.080* (gas saturation-HPLC/UV, measured range 10–50°C, Sonnefeld et al. 1983)

\[ \log (P/\text{Pa}) = 14.385 - 4616.07/(T/\text{K}) ; \text{ temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)} \]

0.473, 0.380 (PGC by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)

log (P/kPa) = 2.88490 – 2635.371/(243.022 + t/°C); temp range 161–300.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.403 (Yamasaki et al. 1984)

\[ \log (P/\text{mmHg}) = 7.7619 - 2637.1/(243.2 + t/°C) ; \text{ temp range 161–300°C (Antoine eq., Dean 1985, 1992)} \]

0.0875* (gas saturation, interpolated-Antoine eq. derived from exptl. data, temp range 34–72°C, Sato et al. 1986)

\[ \ln (P/\text{Pa}) = 17.0935 - 2815.52/(T/\text{K} – 153.984) ; \text{ temp range 307.7–347.5 K (Antoine eq., gas saturation, Sato et al. 1986)} \]

0.0850*, 0.566 (pressure gauge in vacuum cell: solid \( P_S \), supercooled liquid \( P_L \), extrapolated for 25°C from reported Antoine eq., measured temp range 30.03–154.81°C, Sasse et al. 1988)

log (P/\text{mmHg}) = 11.64431 – 4268.644/(262.656 + t/°C); temp range: 30.03–100.08°C (Antoine eq., pressure gauge, Sasse et al. 1988)

\[ \log (P/\text{mmHg}) = 7.74839 - 2641.73/(230.963 + t/°C) ; \text{ temp range 110.06–154.83°C (Antoine eq., pressure gauge, Sasse et al. 1988)} \]

0.474 (\( P_{GC} \) by GC-RT correlation with eicosane as reference standard, Hinckley et al. 1990)

0.793, 0.652(supercooled \( P_L \) converted from literature \( P_S \) with different \( \Delta S_{\text{fus}} \) values, Hinckley et al. 1990)

\[ \log (P/\text{mmHg}) = 53.9382 - 5.322 \times 10^3/(T/\text{K}) - 16.059\log (T/\text{K}) + 4.5696 \times 10^{-3} \times (T/\text{K}) + 8.1430 \times 10^{-13} \times (T/\text{K})^2 ; \text{ temp range 388–870 K (vapor pressure eq., Yaws 1994)} \]

0.407 (supercooled liquid \( P_L \), 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 \( P_L \) from Hinckley et al. 1990; converted to solid \( P_S \) with fugacity ratio F, Passivirta et al. 1999)

log (P1/\text{Pa}) = 11.27 – 3638/(T/\text{K}) (solid, Passivirta et al. 1999)

log (P1/\text{Pa}) = 8.63 – 2614/(T/\text{K}) (supercooled liquid, Passivirta et al. 1999)

log (P1/\text{Pa}) = 14.385 – 4616.07/(T/\text{K}) ; temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)

0.526; 0.194 (supercooled liquid \( P_L \) calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

log (P1/\text{Pa}) = –3492/(T/\text{K}) + 11.43; \( \Delta H_{\text{vap}} = -66.9 \text{ kJ·mol}^{-1} \) (GC-RT correlation, Lei et al. 2002)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

0.086* (25.05°C, transpiration method, measured range 288.7–359.2 K, Verevkin 2004)

\[ \ln \left( \frac{P}{P_a} \right) = \frac{298.47}{R} - \frac{95086.65}{R(T/K)} - \frac{30.2}{R} \cdot \ln \left( \frac{T/K}{298.15} \right) \]; temp range 288.7–359.2 K (transpiration method, Verevkin 2004)

Henry’s Law Constant (Pa m³/mol at 25°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°C, Bamford et al. 1999)

\[ \ln K_{AW} = -\frac{5869.62}{T/K} + 14.193; \Delta H = 48.8 \text{ kJ mol}^{-1}; \text{measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)} \]

\[ \log \left( \frac{H}{(Pa \text{ m}^3/\text{mol})} \right) = 6.97 - \frac{1590}{T/K} \]; temp range 0–40°C (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, \( \log K_{OW} \):

4.18 (Hansch & Leo 1979)
4.12 (Chou & Jurs 1979)
4.18 (HPLC-k’ correlation, Rekker & De Kort 1979)
3.91 (HPLC-k’ 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 ± 0.19, 3.68 ± 0.62 (HPLC-k’ correlation: ODS column; Diol column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°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-C_{A}/C_{A}, measured range 0–40°C, Harner & Bidleman 1998)

\[ \log K_{OA} = -7.74 + 4332/(T/K); \text{temp range 0–40°C (generator column-GC, Harner & Bidleman 1998)} \]

6.83, 6.79 (calculated-S_{oct} and vapor pressure P, quoted lit., Abraham et al. 2001)

Bioconcentration Factor, \( \log BCF \):

3.67 (microorganisms-water, calculated-K_{OW}, Mabey et al. 1982)
2.70 (Daphnia magna, Newsted & Giesy 1987)

Sorption Partition Coefficient, \( \log K_{OC} \):

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 (20°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, $t_{1/2}$:

Volatilization:
Photolysis: half-lives on different atmospheric particulate substrates determined in rotary photoreactor (approx. 25 $\mu$g/g on substrate): $t_{1/2} = 110$ h on silica gel, $t_{1/2} = 62$ h on alumina and $t_{1/2} = 37$ h on fly ash (Behymer & Hites 1985);
photolysis rate $k < 2 \times 10^{-5}$ s$^{-1}$ with $t_{1/2} > 1.6$ d (Kwok et al. 1997):
direct photolysis $t_{1/2} = 7.69$ h (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001)
Photodegradation $k = 9.0 \times 10^{-7}$ 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, $k_{OH}$ for reaction with OH radical, $k_{NO3}$ with NO$_3$ radical and $k_{O3}$ with O$_3$, or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

$k$ (calc) $< 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 3 \times 10^9$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982)
$k_{OH}(calc) = 13.0 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 300 K (SAR structure-activity relationship, Arey et al. 1989,
Atkinson 1989)
$k_{OH}(calc) = 9.90 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculation, Klamt 1996)
$k_{OH}(exptl) = (16 \pm 5) \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, $k_{OH}(calc) = 9.2 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime $\tau = 9$ h; $k_{NO3}(exptl) = (3.5 \pm 1.2) \times 10^{-14}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime $\tau = 1.3$ d; and $k_{O3}(exptl) < 2 \times 10^{-19}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ with a calculated lifetime $\tau > 82$ d at 297 $\pm$ 2 K (relative rate method; calculated-SAR structure-activity relationship, Kwok et al. 1997)
$k_{OH} = 23 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 306–366 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 mg/L are degraded at rates of about 30% per week by microbes (Lee et al. 1984);
$\text{t}_{1/2}(\text{aq. aerobic}) = 768–1440$ h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);
$\text{t}_{1/2}(\text{aq. anaerobic}) = 3072–5760$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated rate constant for bacteria, $3 \times 10^{-9}$ mL cell$^{-1}$ h$^{-1}$ (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:
Air: $t_{1/2} = 6.81$–68.1 h, based on reported rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);
photolysis $t_{1/2} > 1.6$ d; calculated tropospheric lifetimes of 9 h, 1.3 d and > 82d due to reactions with OH radical, NO$_3$ radical and 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: $t_{1/2} = 768–1440$ h, based on aerobic soil die-away test data (Howard et al. 1991).

Groundwater: $t_{1/2} = 1536–2880$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:
Soil: $t_{1/2} = 768–1440$ h, based on aerobic soil die-away test data (Howard et al. 1991);
$t_{1/2} > 50$ d (Ryan et al. 1988).

Biota: elimination $t_{1/2} = 7$ d from rainbow trout (quoted, Meador et al. 1995).
### TABLE 4.1.1.21.1
Reported aqueous solubilities of fluorene at various temperatures

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (S/g·m⁻³)</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>shake flask-UV</td>
</tr>
<tr>
<td>24.6</td>
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<tr>
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<td>5.29</td>
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<td>40.1</td>
<td>3.84, 3.85</td>
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<tr>
<td>47.5</td>
<td>5.59, 5.62</td>
<td>60.5</td>
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<tr>
<td>47.5</td>
<td>5.68</td>
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<td>ΔHfus 19.54 ± 0.13</td>
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<td>73.4</td>
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</tr>
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</table>

\[ \Delta H_{\text{ fus}}/(kJ \cdot mol^{-1}) = 19.54 \]

**Empirical temperature dependence equations:**

Wauchope & Getzen (1972): \( R \ln x = -[H_{\text{ fus}}/(T/K)] + (0.000408)(T/K) - 291.15 \)² – c + b·(T/K)  

May et al. (1978): \(- S/(\mu g/kg) = a \cdot t^4 + b \cdot t^3 + c \cdot t + d \)
FIGURE 4.1.1.21.1 Logarithm of mole fraction solubility (ln 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\ln P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4) \\
\ln P &= A/R - B/[R(T/K)] - (C/R) \cdot \ln [(T/K)/298.15]; \quad R \text{ – gas constant} \quad (5)
\end{align*}
\]

1.

<table>
<thead>
<tr>
<th>Mortimer &amp; Murphy 1923</th>
<th>Stull 1947 summary of literature data</th>
<th>Bradley &amp; Cleasby 1953 effusion</th>
<th>Osborn &amp; Douslin 1975 manometry</th>
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<tr>
<td>isoteniscope-Hg manometer</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
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<td>Bradley &amp; Cleasby 1953</td>
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<td>Effusion</td>
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<td>( t/°C )</td>
<td>( P/Pa )</td>
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<td>25.0</td>
<td>0.080</td>
<td>74.35</td>
<td>13.0</td>
</tr>
<tr>
<td>Eq. 1</td>
<td>P/Pa</td>
<td>Eq. 3</td>
<td>P/Pa</td>
</tr>
<tr>
<td>A</td>
<td>14.385</td>
<td>A</td>
<td>17.0935</td>
</tr>
<tr>
<td>B</td>
<td>4616.07</td>
<td>B</td>
<td>2815.52</td>
</tr>
<tr>
<td>C</td>
<td>–153.984</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eq. 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>110.06</td>
<td>212.5</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>120.04</td>
<td>352.0</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>120.04</td>
<td>353.0</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>129.97</td>
<td>568.6</td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>139.95</td>
<td>894.3</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>149.86</td>
<td>1369</td>
<td></td>
</tr>
<tr>
<td>G</td>
<td>154.81</td>
<td>1683</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>353.2</td>
<td>18.302</td>
<td></td>
</tr>
<tr>
<td>Eq. 2</td>
<td>P/mmHg</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>7.94839</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>2641.73</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>230.963</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temp range: 110–155°C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Eq. 5</td>
<td>P/Pa</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>298.47</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>95086.65</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>30.2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**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

<table>
<thead>
<tr>
<th>Henry’s law constant</th>
<th>log $K_{OA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bamford et al. 1999</td>
<td>Harner &amp; Bidleman 1998</td>
</tr>
<tr>
<td>gas stripping-GC/MS</td>
<td>generator column-GC/FID</td>
</tr>
<tr>
<td>$t/°C$</td>
<td>$H/(Pa \cdot m^3/mol)$</td>
</tr>
<tr>
<td>average</td>
<td></td>
</tr>
<tr>
<td>4.1</td>
<td>1.96, 2.14</td>
</tr>
<tr>
<td>11.0</td>
<td>3.44, 3.65</td>
</tr>
<tr>
<td>18.0</td>
<td>5.81, 6.12</td>
</tr>
<tr>
<td>25.0</td>
<td>9.49, 10.1</td>
</tr>
<tr>
<td>31.0</td>
<td>14.1, 15.4</td>
</tr>
<tr>
<td>25 (exptl)</td>
<td></td>
</tr>
</tbody>
</table>

$ln K_{AW} = A - B/(T/K)$

<table>
<thead>
<tr>
<th>$K_{AW}$</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.193</td>
<td>5870</td>
<td></td>
</tr>
</tbody>
</table>

enthalpy, entropy change:

$\Delta H/(kJ\cdot mol^{-1}) = 48.8 \pm 0.8$

$\Delta S/(J\cdot K^{-1}\cdot mol^{-1}) = 118$

at 25°C

$\Delta H_{OA}/(kJ\cdot mol^{-1}) = 82.9$

$\Delta H_{OA}/(kJ\cdot mol^{-1}) = 82.9$

**FIGURE 4.1.1.21.2** Logarithm of vapor pressure versus reciprocal temperature for fluorene.
FIGURE 4.1.1.21.3 Logarithm of Henry's law constant and $K_{OA}$ 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: C_{14}H_{12}
Molecular Weight: 180.245
Melting Point (°C):
  87 (Lide 2003)
Boiling Point (°C):
  318 (Weast 1982)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  177.1 (Ruelle & Kesselring 1997)
  210.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.246 (mp at 87°C)
Water Solubility (g/m³ or mg/L at 25°C):
  1.092, 4.867 (measured, supercooled liquid value, Miller et al. 1985)
Vapor Pressure (Pa at 25°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 (P_{L}/Pa) = -3711/(T/K) + 11.58; ΔH_{vap} = -71.1 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
  0.032 (24.95°C, transpiration method, measured range 298.1–375.3 K, Verevkin 2004)
  ln (P_{L}/Pa) = 311.78/R – 101590.4/[R(T/K)] – (35.1/R)·ln [(T/K)/298.15]; temp range 298.1–359.2 K (solid, transpiration method, Verevkin 2004)
  ln (P_{L}/Pa) = 330.39/R – 104778.1/[R(T/K)] – (87.5/R)·ln [(T/K)/298.15]; temp range 361.2–375.3 K (liquid, transpiration method, Verevkin 2004)
Henry's Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
  4.97 (calculated, Miller et al. 1985)
  4.63 (calculated-solvatochromic parameters and V_{l}, 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 K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Half-Lives in the Environment:
4.1.1.23 Phenanthrene

Common Name: Phenanthrene
Synonym: o-diphenylethylene, phenanthren
Chemical Name: phenanthrene
CAS Registry No: 85-01-8
Molecular Formula: C_{14}H_{10}
Molecular Weight: 178.229
Melting Point (°C):
99.24 (Lide 2003)
Boiling Point (°C):
340 (Dean 1985; Lide 2003)
Density (g/cm³ at 20°C):
1.174 (Dean 1985)
0.980 (4°C, Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
182.0 (calculated-density, liquid molar volume, Lande & Banerjee 1981)
199.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/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 (74.35, 99.25°C; total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol 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°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.187 (mp at 99.24°C)
Water Solubility (g/m³ or mg/L at 25°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 (27°C, 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 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)
1.18* (shake flask-UV, measured range 24.6–73.4°C, Wauchope & Getzen 1972)
$\ln x = -3890/(T/K) + 4.08 \times 10^{-4} \cdot [(T/K) - 291.15]^2 - 27.9 + 0.0374 \cdot (T/K)$; temp range 24.6–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)
3.03, 2.85 (20°C, 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°C, Schwarz 1977)
S/(µg/kg) = 324.0 + 5.413·(t/°) + 0.8059·(t/°C)² + 0.0025·(t/°C)³; temp range 4–29°C (generator column-HPLC/UV, May et al. 1978)  
0.955* (24.3°C, generator column-HPLC, measured range 4.0–29.9°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°C, Whitehouse 1984)  
1.69 (29°C, shake flask-GC/FID, Stick & 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 S_L (mol/L) = 0.930 – 861.6/(T/K) (supercooled liquid, Passivirta et al. 1999)  
ln x = –2.546051 – 4053/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):  
7773* (230°C, isoteniscope-Hg, measured range 230–340°C, Nelson & Senseman 1922)  
3626* (203.6°C, isoteniscope-Hg manometer, measured range 203.6–346.8°C, Mortimer & Murphy 1923)  
log (P/mmHg) = 7.771 – 2990/(T/K); temp range 203.6–346.8°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)  
133.3* (118.2°C, summary of literature data, temp range 118.2–340.2°C, Stull 1947)  
0.0997 (effusion method, Inokuchi et al. 1952)  
0.0227* (effusion method, Bradley & Cleasby 1953)  
log (P/cmHg) = 10.388 – 4519/(T/K); temp range 36.7–49.65°C (Antoine eq., Bradley & Cleasby 1953)  
log (P/mmHg) = 16.0 – 5008/(T/K); temp range 0–60°C (Knudsen effusion method, Hoyer & Peperle 1958)  
0.464 (extrapolated from Antoine eq. of liquid state P_L, Weast 1972–73)  
log (P/mmHg) = [–0.2185 × 14184.0/(T/K)] + 7.936781; temp range 118.2–340°C (Antoine eq., Weast 1972–73)  
0.159 (extrapolated from Antoine eq. of liquid state P_L, Boublik et al. 1973)  
30.4* (100.0°C, inclined-piston manometry, measured range 100.0–150.0°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 (P/mmHg) = 26.648 – 10484/(T/K); temp range 51.6–90.3°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)  
0.018* (effusion, De Kruif 1980)  
0.0161* (gas saturation-HPLC/UV, Sonnefeld et al. 1983)  
log (P/Pa) = 14.852 – 4962.77/(T/K); temp range 10–50°C (Antoine eq., Sonnefeld et al. 1983)  
0.016 (generator column-HPLC/UV, Wasik et al. 1983)  
0.111, 0.0688 (P_sat by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)  
0.134 (supercooled liquid P_L converted from literature P_S, Bidleman 1984)  
log (P/kPa) = 6.61335 – 2593.134/(224.402 + t/°C); temp range 203.6–346.8°C (Antoine eq. from reported expctl. data, Boublik et al. 1984)  
log (P/kPa) = 6.01392 – 2039.351/(168.569 + t/°C); temp range 230–340°C (Antoine eq. from reported expctl. data, Boublik et al. 1984)  
log (P/mmHg) = 7.26082 – 2379.04/(203.76 + t/°C); temp range 176–379°C (Antoine eq., Dean 1985, 1992)  
0.070 (Yamasaki et al. 1984)  
0.0149 (selected, Howard et al. 1986)
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0.012* (gas saturation, extrapolated-Antoine eq. from expl. data, temp range 49–74°C, Sato et al. 1986)

\[ \ln (P/P_{atm}) = 20.3950 - \frac{49.444}{(T/K - 139.743)}; \text{ temp range: } 322.9–347.8 \text{ K (Antoine eq., gas saturation, Sato et al. 1986)} \]

0.025 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

\[ \log (P/S) = 10.305 - \frac{4444}{T/K}; \text{ temp range 296–315 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]

\[ \log (P/S) = 10.70162 - \frac{4554.38}{T/K}; \text{ temp range 313–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]

\[ \log (P/L) = 6.64812 - \frac{2513.134}{(T/K - 65.345)}; \text{ temp range 373–423 K (Antoine eq., Stephenson & Malanowski 1987)} \]

0.0127, 0.0827 (literature mean P$_S$, supercooled liquid P$_L$, Bidleman & Foreman 1987)

0.111, 0.0556 (P$_{GC}$, GC-RT correlation with different reference standards, Hinckley et al. 1990)

0.134, 0.10 (supercooled liquid P$_L$ converted from literature P$_S$ with different $\Delta S_{fus}$ values, Hinckley et al. 1990)

\[ \log (P/L) = 11.46 - \frac{3716}{T/K}; \text{ temp range 303–333 K (GC-RT correlation, Hinckley et al. 1990)} \]

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)

\[ \log (P/S) = 11.38 - \frac{3842}{T/K}; \text{ temp range 303–333 K (Clausius-Clapeyron eq., Oja & Suuberg 1998)} \]

0.0163 ± 0.004 (gas saturation-HPLC/fluorescence; de Seze et al. 2000)

\[ \log (P/S) = 9.07 - \frac{2982}{(T/K)}; \text{ supercooled liquid, Passivirta et al. 1999) } \]

\[ \log (P/L) = 9.07 - \frac{2982}{(T/K)}; \text{ supercooled liquid, Passivirta et al. 1999) } \]

0.0799; 0.0475 (supercooled liquid P$_L$, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

\[ \log (P/L) = -3768/(T/K) + 11.54; \Delta H_{vap} = -72.2 \text{ kJ mol}^{-1} \text{ (GC-RT correlation, Lei et al. 2002)} \]

0.0202 (solid P$_S$, gas saturation-GC/MS, Mader & Pankow 2003)

\[ \log (P/L) = 0.966; \text{ supercooled liquid P}_L, \text{ calculated from P}_S \text{ assuming } \Delta S_{fus} = 56 \text{ J/mol K, Mader & Pankow 2003) } \]

Henry’s Law Constant (Pa m$^3$/mol at 25°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°C, Alaee et al. 1996)

\[ \ln K_{AW} = 6.0314 - \frac{3524.18}{(T/K)}; \text{ temp range 5.9–34.7°C (gas stripping-GC, Alaee et al. 1996)} \]

3.61 (gas stripping-GC, Shiu & Mackay 1997)

2.90 (gas stripping-HPLC/fluor., De Maagd et al. 1998)

4.29* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)

\[ \ln K_{AW} = -3689.2/(T/K) + 12.75; \Delta H = 47.3 \text{ kJ mol}^{-1}; \text{ measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)} \]

log (H/(Pa m$^3$/mol)) = 8.14 – 2120/(T/K) (Passivirta et al. 1999)

3.85 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 2001)

log $K_{AW} = 2.417 - 1530/(T/K)$ (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°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 ± 0.15 (recommended, Sangster 1989, 1993)
- 4.374 ± 0.034, 4.562 ± 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 (26°C, 4°C, quoted, Piatt et al. 1996)
- 4.48 ± 0.19, 4.54 ± 0.61 (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 & Schrädter 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 $K_{OA}$ at 25°C or as indicated and reported temperature dependence equation:

- 7.45 (calculated, Finizio et al. 1997)
- 7.57*; 7.41 (generator column-GC; calculated-concn ratio $C_O/C_A$, measured range 0–40°C, Harner & Bidleman 1998)

$log K_{OA} = -5.62 + 3942/(T/K)$; temp range 0–40°C, $\Delta H_{OA} = 63.3 \text{ kJ/mol}$ (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 (fathead minnow, Carlson et al. 1978)
- 2.51 (Daphnia pulex, Southworth et al. 1978)
- 2.57 (kinetic estimation, Southworth et al. 1978)
- 3.80 (mixed microbial population, Steen & Karickhoff 1981)
- 4.28 (P. hoyi, Eadie et al. 1982)
- 3.67 (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 (Chlorella fusca; Geyer et al. 1984)
- 2.51 (fish, Govers et al. 1984)
- 2.97, 3.25, 3.25 (activated sludge, algae, fish, Freitag et al. 1985)
- 4.18; 4.28 (P. hoyi of Lake Michigan interstitial waters; of high sediment study site, Landrum et al. 1985)
- 2.51 (Daphnia magna, Newsted & Giesy 1987)
- 3.21 (10–20°C, h. limbata, rate constant ratio $k_1/k_2$, Landrum & Poore 1988)
- 4.45; 3.77; 3.43 (4°C, P. hoyi; S. heringiana; Mysis relicta, quoted, Landrum & Poore 1988)
- 0.756, 1.487 (Polychaete sp, Capitella capitata, Bayona et al. 1991)
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Sorption Partition Coefficient, log $K_{OC}$ at 25°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 $C_{sed}/C_W$; 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) (4°C, low organic carbon sediment $f_{OC} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
4.13  (range 4.06–4.19); 3.48 (range 3.47–3.48) (26°C, low organic carbon sediment $f_{OC} = 0.0002$, batch equilibrium; column exptl., Piatt et al. 1996)
4.65; 4.81 ± 0.16  (humic acid, HPLC-k′ correlation; quoted lit., Nielsen et al. 1997)
2.42–2.56  (5 soils, 20°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 ± 0.088 (soils: Woodburn soil, Elliot soil, Marlette soil, Piketon soil, Anoka soil, batch equilibrium-sorption isotherms-HPLC-fluorescence, Cho et al. 1998)
4.38, 4.45, 4.53, 4.33, 4.42, 4.62, 4.64 ± 0.087 (sediments: Lake Michigan, Mississippi River, Massachusetts Bay, Spectacle Island, Peddocks Island, Port Point Channel, batch equilibrium-sorption isotherms-HPLC-fluorescence, Cho et al. 1998)
4.48  (4.46–4.50), 4.22 (4.20–4.23) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maagd et al. 1998)
3.67; 3.29, 4.04, 3.27, 4.37, 4.21 (calculated-$K_{OW}$; HPLC-screening method with different LC-columns, Szabo et al. 1999)
3.31–6.02  (range, calculated from sequential desorption of 11 urban soils; Krauss & Wilcke 2001)
5.34; 5.23, 4.82, 4.98 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic 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 OC ≥ 0.1%, OC ≥ 0.5%, average, Delle Site 2001)
4.34  (average values for sediment OC ≥ 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)
Environmental Fate Rate Constants, k, or Half-Lives, $t_\text{½}$:

Volatilization: half-lives from solution: 97, 108 min (exptl., calculated, Mackay et al. 1983).

Photolysis: calculated $t_\text{½} = 8.4$ h for direct sunlight photolysis at 40°N latitude of midday in midsummer, near surface water and $t_\text{½} = 59$ d (inland water) and $t_\text{½} = 69$ d for inland water with sediment partitioning in a 5-m deep inland water body (Zepp & Schlotzhauer 1979)

$\text{t}_\text{½} = 3$ h, atmospheric and aqueous half-life, based on measured aqueous photolysis quantum yields and calculated for midday summer sunlight at 40°N latitude and $t_\text{½} = 25$ h after adjusting for approximate winter sunlight intensity (Howard et al. 1991);

half-lives on different atmospheric particulate substrates (appr. 25 µg/g on substrate): $t_\text{½} = 150$ h on silica gel, $t_\text{½} = 45$ h on alumina and $t_\text{½} = 49$ h on fly ash (Behymer & Hites 1985);

$k = 0.11$ h$^{-1}$ with $t_\text{½} = 6.3$ h in distilled water (Fukuda et al. 1988);

photodegradation $k = 6.53 \times 10^{-3}$ min$^{-1}$ and $t_\text{½} = 1.78$ h in methanol-water (2:3, v/v) solution with an initial concn of 5.0 ppm under high pressure mercury lamp or sunlight (Wang et al. 1991)

$k(\text{expt}) = 0.00653$ min$^{-1}$ pseudo-first-order direct photolysis rate constant with the calculated $t_\text{½} = 1.78$ h and the predicted $k = 0.00165$ min$^{-1}$ calculated by QSPR, in aqueous solution when irradiated with a 500-W medium pressure mercury lamp (Chen et al. 1996);

photodegradation under atmospheric conditions: $k = (4.49 \pm 0.68) \times 10^{-5}$ s$^{-1}$ and $t_\text{½} = (4.29 \pm 0.57)$ h in diesel particulate matter, $k = (2.11 \pm 0.04) \times 10^{-5}$ s$^{-1}$ and $t_\text{½} = (9.1 \pm 0.19)$ h in diesel particulate matter/soil mixture, and $t_\text{½} = 17 - 4.97$ h in various soil components using a 900-W photo-irradiator as light source; $k = (3.17 \pm 0.06) \times 10^{-5}$ s$^{-1}$ and $t_\text{½} = (60.63 \pm 1.33)$ h in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

photodegradation $k = 0.09 \times 10^{-4}$ 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, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO$_3$ radical and $k_{\text{O}_3}$ with O$_3$ or as indicated, *data at other temperatures see reference:

$k_{\text{(aerial)}} = 0.01$ L M$^{-1}$ s$^{-1}$ with $t_\text{½} = 8 \times 10^6$ d (Callahan et al. 1979)

$k_{\text{(calc)}} < 360$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k < 36$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982)

$k = (1.33 - 1.57) \times 10^4$ dm$^3$ mol$^{-1}$ s$^{-1}$ over the pH range 1–7 for the reaction with O$_3$ in water at 25°C, $t_\text{½} = 0.44$ s in presence of 10$^{-4}$ M ozone at pH 7 (Butković et al. 1983)

$k_{\text{OH}} = 3.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 ± 1 K, $k_{\text{OH}} = 2.8 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 319 ± 1 K (relative rate method, Biermann et al. 1985)

$k_{\text{OH}} = 3.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (review, Atkinson 1989)

$k_{\text{OH}} = 25.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = 27 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K, measured range 346–386 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);

$t_{\text{½(aerobic)}} = 384–4800$ h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991); $k = 0.0447$ d$^{-1}$ with $t_{\text{½}} = 16$ d for Kidman sandy loam and $k = 0.0196$ d$^{-1}$ with $t_{\text{½}} = 35$ d for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990);

$t_{\text{½(an aerobic)}} = 1536–19200$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

$\tau = 4 \text{ d}$ in inorganic solution and $\tau = 11 \text{ d}$ 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 creosote-
contaminated marine sediments with nitrate- and sulfate-reducers respectively under anaerobic conditions
in a fluidized bed reactor (Rockne & Strand 1998)

first-order $k = 0.033$ to 0.139 L mg$^{-1}$ 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, $1.6 \times 10^{-2}$ mL cell$^{-1}$ h$^{-1}$ (Paris et al. 1980; quoted, Mabey et al. 1982)

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 203 \text{ h}^{-1}; k_2 = 0.543 \text{ h}^{-1}$ (Daphnia pulex, Southworth et al. 1978)

$log k_1 = 2.31 \text{ h}^{-1}; log k_2 = -0.27 \text{ h}^{-1}$ (Daphnia pulex, as per the correlation of Mackay & Hughes 1984,
Hawker & Connell 1986)

$k_1 = 129.0 \text{ mL g}^{-1} \text{ h}^{-1}; k_2 = 0.0046 \text{ h}^{-1}$ (4°C, p. hoyi, Landrum 1988; quoted, Landrum & Poore 1988)

$k_1 = 52.5 \text{ h}^{-1}; k_2 = 0.032 \text{ h}^{-1}$ (10–20°C, H. limbata, Landrum & Poore 1988)

$k_1 = 94.0 \text{ h}^{-1}; k_2 = 0.016 \text{ h}^{-1}$ (4°C, S. heringianus, quoted, Landrum & Poore 1988)

$k_1 = 32.0 \text{ h}^{-1}; k_2 = 0.012 \text{ h}^{-1}$ (4°C, Mysis relicta, quoted, Landrum & Poore 1988)

$k_1 = 8.8 \text{ mg g}^{-1} \text{ h}^{-1}; k_2 = 0.045 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $\tau = 6 \text{ h}$ with a steady-state concn of tropospheric ozone of $2 \times 10^{-9} \text{ M}$ in clean air (Butkovic et al. 1983)

t$_{1/2} = 2.01$–20.1 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, $t_{1/2} = 8.4 \text{ h}$ for direct photochemical transformation at
latitude 40°N, midday, midsummer with $t_{1/2} = 59 \text{ d}$ (no sediment-water partitioning), $t_{1/2} = 69 \text{ d}$ (with sediment-
water partitioning) on direct photolysis in a 5-m deep inland water body (Zepp & Schlotzhauer 1979);
t$_{1/2} = 0.44 \text{ s}$ in presence of $10^{-4} \text{ M}$ ozone at pH 7 (Butkovic et al. 1983);
calculated $t_{1/2} = 59 \text{ d}$ under sunlight for summer at 40°N latitude (Mill & Mabey 1985);
t$_{1/2} = 3$–25 h, based on aqueous photolysis half-life (Howard et al. 1991);
photoysis $t_{1/2} = 1.78 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp
(Chen et al. 1996).

Groundwater: $t_{1/2} = 768$–9600 h, based on estimated unacclimated aqueous aerobic biodegradation half-life
(Howard et al. 1991).

Sediment: reduction $t_{1/2}(\text{est.}) = 1196 \text{ h}$, $t_{1/2}(\text{exptl}) = 825 \text{ h}$ for chemical available phenanthrene and $t_{1/2} = 151 \text{ h}$ for
bioavailable phenanthrene in Lake Michigan sediments at 4°C. The average uptake clearance from sediment was
(0.041 ± 0.023)g of dry sediment·g$^{-1}$ of organism·h$^{-1}$, and the rate constants to
to become biologically unavailable was (0.0055 ± 0.003) h$^{-1}$ resulting a bioavailable $t_{1/2} = 126 \text{ h}$ (Landrum 1989);
formation $t_{1/2} = 8.6 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 2.5$–26 d (Sims & Overcash 1983; quoted, Bulman et al. 1987);
t$_{1/2} = 9.7 \text{ d}$ for 5 mg/kg treatment and $t_{1/2} = 14 \text{ d}$ for 50 mg/kg (Bulman et al. 1987);
biodegradation $k = 0.0447 \text{ d}^{-1}$ with $t_{1/2} = 16 \text{ d}$ in Kidman sandy loam soil and $k = 0.0196 \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$
in McLaurin sandy loam soil (Park et al. 1990);
biodegradation $t_{1/2} = 11 \text{ d}$ in Kendaia soil (Manilal & Alexander 1991);
t$_{1/2} = 384$–4800 h, based on aerobic soil die-away test data (Howard et al. 1991);
t$_{1/2} > 50 \text{ d}$ (Ryan et al. 1988);
t$_{1/2} = 0.4$–26 wk, 5.7 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: depuration $t_{1/2} = 40.9 \text{ h}$ in S. heringianus (Frank et al. 1986);

elimination $t_{1/2} = 9 \text{ d}$ from rainbow trout, $t_{1/2} = 8.4 \text{ d}$ from clam Mya arenaria, $t_{1/2} = 1.9 \text{ d}$ from mussel Mytilus edulis;
$t_{1/2} = 7 \text{ d}$ from polychaete Abarenicola pacifica, $t_{1/2} = 3.4 \text{ d}$ from Oyster, $t_{1/2} = 0.9 \text{ d}$ from shrimp,
$t_{1/2} = 4.8 \text{ d}$ from polychaete Nereis virens, $t_{1/2} = 6.1 \text{ d}$ from clam Mercenaria mercenaria (Meador et al. 1995).
### TABLE 4.1.1.23.1
Reported aqueous solubilities of phenanthrene at various temperatures

1.

<table>
<thead>
<tr>
<th></th>
<th>Wauchope &amp; Getzen 1972</th>
<th>Schwarz 1977</th>
<th>May et al. 1978a</th>
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<td>shake flask-fluorescence</td>
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<td>S/g·m⁻³</td>
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<td>2.44, 2.45</td>
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<td>65.1</td>
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<td>65.1</td>
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<td>(\Delta H_{\text{ fus}}) 16.28 ± 0.08</td>
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<tr>
<td>70.7</td>
<td>12.4</td>
<td>(10^b)</td>
<td>3.74 ± 0.13</td>
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<td>70.7</td>
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<td>c</td>
<td>27.9 ± 0.4</td>
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<td>73.4</td>
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\(\Delta H_{\text{ fus}}/(\text{kJ mol}^{-1}) = 16.28\)

<table>
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\(\Delta H_{\text{ fus}}/(\text{kJ mol}^{-1}) = 16.28\)

**Empirical temperature dependence equations:**

Wauchope & Getzen (1972): \(R \cdot \ln x = -[H_{\text{ fus}}/(T/K)] + (0.000408)(T/K) - 291.15] - c + b(T/K)\) (1)

May et al. (1978): \(S/(\mu g/kg) = a \cdot t^3 + b \cdot t^{1/2} + c \cdot t + d\) (2)
TABLE 4.1.1.23.1 (Continued)

2.

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temp dependence eq. 2

S µg/kg
a 0.0025
b 0.8059
c 5.412
d 324

\( \Delta H_{sol}/(kJ \cdot mol^{-1}) = 34.81 \)

for temp range 5–30°C

FIGURE 4.1.1.23.1 Logarithm of mole fraction solubility (ln 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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \quad (1a) \\
\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \quad (2a) \\
\log P &= A - \frac{B}{C + T/K} \quad (3) \\
\ln P &= A - \frac{B}{C + T/K} \quad (3a) \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

1. **Nelson & Senseman 1922**

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2. **Hoyer & Peperle 1958**

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<tr>
<td>115.0</td>
<td>73.5</td>
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<td>120.0</td>
<td>95.9</td>
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<tr>
<td>125.0</td>
<td>124.79</td>
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<tr>
<td>130.0</td>
<td>161.05</td>
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<tr>
<td>135.0</td>
<td>207.18</td>
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<tr>
<td>140.0</td>
<td>264.91</td>
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<tr>
<td>145.0</td>
<td>335.30</td>
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<tr>
<td>150.0</td>
<td>420.76</td>
</tr>
</tbody>
</table>

\[\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 95.90\]

\[\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 90.5\]
### Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

**TABLE 4.1.1.23.2 (Continued)**

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<td></td>
<td>efusion</td>
<td>inclined-piston manometry</td>
<td>gas saturation-GC</td>
<td>effusion</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td></td>
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</tr>
<tr>
<td>3.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\Delta H_v/(kJ \text{ mol}^{-1}) = \\
\text{at 398.15 K} \quad 68.58 \\
\text{at tp} \quad 70.79
\]

\[
\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 87.24 \\
\text{at tp}
\]

\[
\Delta H_{fus}/(kJ \text{ mol}^{-1}) = 16.44
\]

### 3.

<table>
<thead>
<tr>
<th></th>
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</tr>
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<tbody>
<tr>
<td></td>
<td>generator column-HPLC</td>
<td>gas saturation-electrobalance</td>
<td>Knudsen effusion</td>
</tr>
<tr>
<td>t/°C</td>
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<td>P/Pa</td>
<td>t/°C</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>10.35</td>
<td>322.9</td>
<td>0.340</td>
<td>30.34</td>
</tr>
<tr>
<td>10.35</td>
<td>324.6</td>
<td>0.420</td>
<td>37.22</td>
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<td>10.35</td>
<td>328.5</td>
<td>0.655</td>
<td>40.77</td>
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<td>10.35</td>
<td>333.0</td>
<td>1.05</td>
<td>44.79</td>
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<tr>
<td>18.85</td>
<td>335.2</td>
<td>1.34</td>
<td>40.1</td>
</tr>
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<td>18.85</td>
<td>337.8</td>
<td>1.73</td>
<td>59.78</td>
</tr>
<tr>
<td>18.85</td>
<td>339.5</td>
<td>2.03</td>
<td></td>
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<td>29.5</td>
<td>343.2</td>
<td>2.98</td>
<td>eq. 1a</td>
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<td>29.5</td>
<td>346.0</td>
<td>3.75</td>
<td>A</td>
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<td>29.5</td>
<td>347.8</td>
<td>4.42</td>
<td>B</td>
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<tr>
<td>38.65</td>
<td>0.0917</td>
<td>eq. 3a</td>
<td>P/Pa</td>
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<tr>
<td>3865</td>
<td>0.0889</td>
<td>A</td>
<td>20.3950</td>
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<tr>
<td>38.65</td>
<td>0.0849</td>
<td>B</td>
<td>3931.20</td>
</tr>
<tr>
<td>38.80</td>
<td>0.0863</td>
<td>C</td>
<td>-139.743</td>
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<tr>
<td>38.80</td>
<td>0.0844</td>
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<tr>
<td>38.88</td>
<td>0.0902</td>
<td></td>
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</tr>
<tr>
<td>38.90</td>
<td>0.0902</td>
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<tr>
<td>38.90</td>
<td>0.0922</td>
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<tr>
<td>38.90</td>
<td>0.0906</td>
<td></td>
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<tr>
<td>25.0</td>
<td>0.0161</td>
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</tr>
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</table>

\[
\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 95.0
\]

\[
\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 96.5
\]

\[
\Delta H_{sub}/(kJ \text{ mol}^{-1}) = 95.0
\]
**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

\[
\ln K_{AW} = A - B/(T/K) \quad (1) \quad \log K_{AW} = A - B/(T/K) \quad (1a)
\]

\[
\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \quad \log (1/K_{AW}) = A - B/(T/K) \quad (2a)
\]

\[
\ln (k_H/\text{atm}) = A - B/(T/K) \quad (3)
\]

\[
\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K) \quad (4) \quad \ln [H/(\text{atm·m}^3/\text{mol})] = A - B/(T/K) \quad (4a)
\]

\[
K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2 \quad (5)
\]

**Henry's law constant**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.9</td>
<td>1.81</td>
<td>31.0</td>
<td>14,1293</td>
</tr>
<tr>
<td>10.4</td>
<td>2.99</td>
<td>11.0</td>
<td>1.53, 1.67</td>
</tr>
<tr>
<td>15.0</td>
<td>3.06</td>
<td>18.0</td>
<td>2.55, 2.70</td>
</tr>
<tr>
<td>20.2</td>
<td>3.66</td>
<td>25.0</td>
<td>4.08, 4.51</td>
</tr>
<tr>
<td>25.7</td>
<td>4.73</td>
<td>31.0</td>
<td>5.97, 6.82</td>
</tr>
<tr>
<td>30.2</td>
<td>5.54</td>
<td>31.0</td>
<td>5.97, 6.82</td>
</tr>
<tr>
<td>34.7</td>
<td>7.90</td>
<td>ln K_{AW} = A - B/(T/K)</td>
<td>A</td>
</tr>
</tbody>
</table>

**log K_{OA}**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>log K_{OA}</th>
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<tbody>
<tr>
<td>0</td>
<td>8.808</td>
</tr>
<tr>
<td>10</td>
<td>8.267</td>
</tr>
<tr>
<td>20</td>
<td>7.898</td>
</tr>
<tr>
<td>30</td>
<td>7.418</td>
</tr>
<tr>
<td>40</td>
<td>6.926</td>
</tr>
</tbody>
</table>

**Alaee et al. 1996**

**Bamford et al. 1999**

**Harner & Bidleman 1998**

Experimental data

Stull 1947

Hoyer & Peperle 1958 (0 to 60 °C)

m.p. = 99.24 °C

b.p. = 340 °C

enthalpy of volatilization:

\[
\Delta H_{\text{vol}}/(\text{kJ·mol}^{-1}) = 29.3 \text{ at } 20^\circ C
\]

enthalpy of phase change

\[
\Delta H_{\text{OA}}/(\text{kJ·mol}^{-1}) = 75.5
\]

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FIGURE 4.1.1.23.3 Logarithm of Henry's law constant and $K_{OA}$ versus reciprocal temperature for phenanthrene.
4.1.1.24 1-Methylphenanthrene

Common Name: 1-Methylphenanthrene

Chemical Name: 1-methylphenanthrene

CAS Registry No: 832-69-6

Molecular Formula: C_{15}H_{12}

Molecular Weight: 192.256

Melting Point (°C):
123  (Weast 1982–83; Lide 2003)

Boiling Point (°C):
354  (Lide 2003)

Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
188.0  (Ruelle & Kesselring 1997)
221.4  (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):

Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F: 0.109 (mp at 123°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated *, are compiled at the end of this section):
0.255*  (24.1°C, generator column-HPLC/UV, measured range 6.6–29.9°C, May et al. 1978a, 1983)
0.269  (generator column-HPLC, May et al. 1978b)

S/(µg/kg) = 55.42 + 6.8016·(t/°) – 0.1301·(t/°C)² + 0.0080·(t/°C)³; temp range 6.6–29.9°C (generator column-HPLC/UV, May et al. 1978)

Vapor Pressure (Pa at 25°C and the reported temperature dependence equation):
0.0186; 0.0160  (supercooled liquid \( P_L \), calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

\[ \log (P/L/Pa) = -3987/(T/K) + 11.64; \Delta H_{\text{vap}} = -76.3 \text{kJ·mol}^{-1} \]  (GC-RT correlation, Lei et al. 2002)

Henry’s Law Constant (Pa m³/mol at 25°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°C, Bamford et al. 1999)

\[ \ln K_{AW} = -4257.88/(T/K) + 8.0587, \Delta H = 35.4 \text{kJ·mol}^{-1}; \text{measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)} \]

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
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 \( K_{\text{OA}} \):

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{\text{OC}} \):

Environmental Fate Rate Constants, k or Half-Lives, \( t_{1/2} \):

Volutilization:
Photolysis: photodegradation of 5 ppm initial concentration in methanol-water (3:7, v/v) by high pressure mercury lamp or sunlight with a rate constant \( k = 1.84 \times 10^{-3} \text{min}^{-1} \) and \( t_{1/2} = 6.27 \text{h} \) (Wang et al. 1991);
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

pseudo-first-order direct photolysis \( k_{\text{expt}} = 0.00184 \text{ min}^{-1} \) with the calculated \( t_{1/2} = 6.27 \text{ h} \) and the predicted \( k = 0.0026 \text{ min}^{-1} \) calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996); direct photolysis \( t_{1/2} = 3.10 \text{ h} \) (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).

Hydrolysis:
Oxidation:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

Half-Lives in the Environment:
Air: direct photolysis \( t_{1/2} = 3.10 \text{ h} \) (predicted-QSPR) in atmospheric aerosol (Chen et al. 2001).
Surface water: photolysis \( t_{1/2} = 6.27 \text{ h} \) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).
Groundwater:
Sediment:
Soil:
Biota: elimination \( t_{1/2} = 6.7 \text{ d} \) from Oyster, 6.0 d from clam *Mercenaria 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

\[
S/(\mu g/kg) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)
\]

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<tbody>
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<td>generator column-HPLC</td>
<td>generator column-HPLC</td>
<td>generator column-HPLC</td>
<td>gas stripping-GC/MS</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>S/g·m⁻³</strong></td>
</tr>
<tr>
<td>6.6</td>
<td>0.0952</td>
<td>25.0</td>
<td>0.269</td>
</tr>
<tr>
<td>8.9</td>
<td>0.114</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14.0</td>
<td>0.147</td>
<td>temp dependence eq. 1</td>
<td></td>
</tr>
<tr>
<td>19.2</td>
<td>0.193</td>
<td>S/μg/kg</td>
<td></td>
</tr>
<tr>
<td>24.1</td>
<td>0.255</td>
<td>a</td>
<td>0.0080</td>
</tr>
<tr>
<td>26.9</td>
<td>0.304</td>
<td>b</td>
<td>0.1301</td>
</tr>
<tr>
<td>29.9</td>
<td>0.355</td>
<td>c</td>
<td>6.8016</td>
</tr>
<tr>
<td></td>
<td></td>
<td>d</td>
<td>55.42</td>
</tr>
</tbody>
</table>

data of May et al. 1978a temp dependence eq. 1

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<th><strong>S</strong>/μg/kg</th>
<th><strong>a</strong></th>
<th><strong>b</strong></th>
<th><strong>c</strong></th>
<th><strong>d</strong></th>
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<td>measured between 5–30°C</td>
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<tr>
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<td>0.0080</td>
<td>0.1301</td>
<td>6.8016</td>
<td>55.42</td>
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</table>

data of May 1980 fitted to temp dependence eq. 1

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<th><strong>b</strong></th>
<th><strong>c</strong></th>
<th><strong>d</strong></th>
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<td>0.0074</td>
<td>-0.0858</td>
<td>5.785</td>
<td>62.9</td>
</tr>
<tr>
<td>ln ( K_{AW} ) = A – B/(T/K)</td>
<td>A</td>
<td>8.0587</td>
<td>B</td>
<td>4257.88</td>
</tr>
</tbody>
</table>

enthalpy, entropy change:

\[
\Delta H/(kJ·mol⁻¹) = 35.4 ± 1.9 \\
\Delta S/(J·K⁻¹·mol⁻¹) = 67 \\
at 25°C
\]
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: C_{14}H_{10}
Molecular Weight: 178.229

Melting Point (°C):
- 215.76 (Lide 2003)

Boiling Point (°C):
- 339.9 (Lide 2003)

Density (g/cm³ at 20°C):
- 1.25 (27°C, Dean 1985)
- 1.28 (25°C, Lide 2003)

Molar Volume (cm³/mol):
- 139 (calculated-density, liquid molar volume, Lande & Banerjee 1981)
- 196.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
- 28.83 (Parks & Huffman 1931)
- 28.87 (Tsonopoulos & Prausnitz 1971; Ruelle & Kesselring 1997)
- 29.37 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol 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°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0134 (mp at 215.76°C)
- 0.0101 (calculated, ΔS_{fus} = 58.6 J/mol K, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°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 (27°C, 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 (20°C, shake flask-UV, Eisenbrand & Baumann 1970)
- 0.040 (shake flask-UV, Eisenbrand & Baumann 1970)
- 0.171, 0.0392 (20°C, HPLC-relative retention correlation, different stationary or mobile phases, Locke 1974)
- 0.075* (extrapolated value, shake flask-UV, measured range 25–74.7°C, Wauchope & Getzen 1972)

R ln x = –6930/(T/K) + 4.08 × 10⁻⁴[(T/K) – 291.15]² – 19.3 + 0.0181·(T/K), temp range 35.4–73.4°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 (Rossi 1977; Neff 1979)
- 0.041* (shake flask-UV, measured range 8.6–31.3°C, Schwarz 1977)
- 0.074 (Lu et al. 1978)
- 0.0446* (generator column-HPLC/UV, measured range 5.2–29.3°C, May et al. 1978)
- 0.0434* (24.6°C, generator column-HPLC, measured range 5.2–28.7°C, May 1980)
\[
S/(\mu g/kg) = 8.21 + 0.8861 \cdot (t/°C) + 0.0097 \cdot (t/°C)^2 + 0.0013 \cdot (t/°C)^3; \text{ temp range 5.2–29.3°C (generator column-HPLC/UV, May et al. 1978)}
\]

0.033 \quad (20°C, generator column-fluorescence, Hashimoto et al. 1982)

0.0434* \quad (24.6°C, generator column-HPLC, measured range 5.6–29.3°C, May et al. 1983)

0.030, 0.051 \quad (generator column-HPLC/UV, Swann et al. 1983)

0.04257* \quad (generator column-spectrofluorimetry, measured range 10–30°C, Velapoldi et al. 1983)

0.0446 \quad (generator column-HPLC/UV, Wasik et al. 1983)

0.066 \quad (average lit. value, Pearlman et al. 1984)

0.0698 \quad (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.0442* \quad (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)

0.0446 \quad (vapor saturation-UV, Akiyoshi et al. 1987)

0.066 (average lit. value, Pearlman et al. 1984)

0.0698 \quad (generator column-HPLC/fluorescence, Walters & Luthy 1984)

0.0442* \quad (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)

0.0446 \quad (vapor saturation-UV, Akiyoshi et al. 1987)

0.0434* \quad (20°C, shake flask/UV, ring test, Kishi & Hashimoto 1989)

0.062* \quad (recommended, IUPAC Solubility Data Series, Shaw 1989)

0.070 \quad (23°C, shake flask-HPLC/fluorescence, Pinal et al. 1991)

0.058 \quad (generator column-HPLC, Vadas et al. 1991)

0.0488 \quad (dialysis tubing equilibration-GC, Etzweiler et al. 1995)

0.043 \quad (20°C, shake flask-HPLC, Haines & Sandler 1996)

0.0796; 0.138, 0.0743 \quad (quoted, exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

Vapor Pressure (Pa at 25°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 (220°C, isoteniscope-Hg, measured range 220–342°C, Nelson & Senseman 1922)

6399* \quad (223.3°C, isoteniscope-Hg manometer, measured range 223.3–340.5°C, Mortimer & Murphy 1923)

log (P/mmHg) = 10.972 – 4595/(T/K); temp range 100–210°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)

log (P/mmHg) = 7.910 – 3093/(T/K); temp range 223.2–340.5°C (Antoine eq., static isoteniscope method, Mortimer & Murphy 1923)

133.3* \quad (145.0°C, summary of literature data, temp range 145.0–342.0°C, Stull 1947)

log (P/mmHg) = 12.0072 – 5102.6/(T/K); temp range 378–398 K (Rodebush gauge, Sears & Hopke 1949)

8.31 × 10–4 (effusion method, Inokuchi et al. 1952; quoted, Bidleman 1984)

8.31 × 10–4 (effusion method, Bradley & Cleasby 1953)

log (P/mmHg) = 12.0072 – 5102.6/(T/K); temp range 378–398 K (Rodebush gauge, Sears & Hopke 1949)

log (P/mmHg) = 12.0072 – 5102.6/(T/K); temp range 378–398 K (Rodebush gauge, Sears & Hopke 1949)

3.60 × 10–3 (effusion method, Inokuchi et al. 1952; quoted, Bidleman 1984)

8.31 × 10–4 (effusion method, Bradley & Cleasby 1953)

log (P/mmHg) = 12.0072 – 5102.6/(T/K); temp range 378–398 K (Rodebush gauge, Sears & Hopke 1949)

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Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

\[
\log (P/\text{mmHg}) = 10.0216 - 4397.60/(T/K); \text{ temp range } 290.1-358 \text{ K (Knudsen method, Wiedemann & Vaughan 1969, Wiedemann 1972)}
\]

\[
\log (P/\text{mmHg}) = 7.67401 - 2819.63/(247.02 + t/°C); \text{ temp range: } 175.5-380°C (liquid state, Antoine eq., Zwolinski & Wilhoit 1971)
\]

\[
\log (P/\text{mmHg}) = -0.2185 \times 16823.6/(T/K) + 8.70760; \text{ temp range } 100-600°C (Antoine eq., Weast 1972-73)
\]

\[
1.113 \times 10^{-3} \text{ (Knudsen effusion weight-loss method, extrapolated Malaspina et al. 1973)}
\]

\[
\log (P/\text{mmHg}) = 12.616 - 5277/(T/K); \text{ temp range } 352.7-432.3 \text{ K (Knudsen method, Malaspina et al. 1973)}
\]

\[
1.47 \times 10^{-5} \text{ (effusion method, Taylor & Crooks 1976)}
\]

\[
9.04 \times 10^{-4} \text{ (gas saturation, extraplated-Clapeyron eq., measured range } 85.25-119.95°C, \text{ Macknick & Prausnitz 1979)}
\]

\[
\log (P/\text{mmHg}) = 26.805 - 11402/(T/K); \text{ temp range } 85.25-119.95°C (Clapeyron eq., gas saturation, Macknick & Prausnitz 1979)
\]

\[
7.50 \times 10^{-4} \text{ (effusion methods, extrapolated, measured range } 64.44-87.74°C, \text{ De Kruif 1980)}
\]

\[
4.90 \times 10^{-4} \text{ (calculated-TSA, Amidon & Anik 1981)}
\]

\[
1.83 \times 10^{-3} \text{ (gas saturation, extrapolated-Antoine eq., measured range } 50-85°C, \text{ Grayson & Fosbraey 1982)}
\]

\[
1.44 \times 10^{-3} \text{ (gas saturation, extrapolated-Antoine eq. measured range } 80-125°C, \text{ Bender et al. 1983)}
\]

\[
\ln (P/Pa) = 17.88 - 5359/(T/K); \text{ temp range } 313-363 \text{ K (Clausius-Clapeyron eq., Hansen & Eckert 1986)}
\]

\[
1.14 \times 10^{-3} \text{ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)}
\]

\[
\log (P S/kPa) = 11.76139 - 5315.532/(T/K); \text{ temp range } 313-363 \text{ K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)}
\]

\[
\log (P S/kPa) = 10.75544 - 3642/(T/K); \text{ temp range } 504-615 \text{ K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
5.73 \times 10^{-4}; 5.60 \times 10^{-3} \text{ (literature mean solid } P S, \text{ supercooled liquid } P L, \text{ Bidleman & Foreman 1987)}
\]

\[
0.0865 \text{ (supercooled liquid } P L, \text{ converted from literature } P S \text{ with } \Delta S_{fus} \text{ Bidleman 1984)}
\]

\[
\log (P_0/\text{Pa}) = 11.18 - 3642/(T/K); \text{ temp range } 504-615 \text{ K (liquid, Antoine eq.-IV, Stephenson & Malanowski 1987)}
\]

\[
0.0049-0.00125; 0.000925-0.00129 \text{ (quoted lit. values by: calculation; from GC-RT relation, Delle Site 1997)}
\]

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8.69 × 10^{-4} (Knudsen effusion, extrapolated-Antoine eq. derived from exptl. data, temp range 30–60°C, Oja & Suuberg 1998)

\[
\log (P/Pa) = 33.281 - 12024/(T/K); \text{ temp range 318–363 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)}
\]

9.01 × 10^{-2}; 9.08 × 10^{-4} (quoted supercooled liquid P_L from Hinckley et al. 1990; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

\[
\log (P_P/Pa) = 11.66 - 4380/(T/K) \quad \text{ (solid, Passivirta et al. 1999)}
\]

\[
\log (P/Pa) = 33.281 - 12024/(T/K); \text{ temp range 318–363 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)}
\]

0.0724; 0.0442 (supercooled liquid P_L, calibrated GC-RT correlation; GC-RT correlation, Lei et al. 2002)

\[
\Delta H_{\text{vap.}} = -72.4 \text{ kJ mol}^{-1} \quad \text{ (GC-RT correlation, Lei et al. 2002)}
\]

0.0014 (solid P_S, gas saturation-GC/MS, Mader & Pankow 2003)

0.0922 (supercooled liquid P_L, calculated from P_S assuming \( \Delta S_{\text{fus}} = 56 \text{ J mol}^{-1} \text{ K} \), Mader & Pankow 2003)

\[
\ln (P/Pa) = (34.199 \pm 0.641) - (12339 \pm 229)/(T/K); \text{ temp range 348–368 K (gas stripping-GC, Bamford et al. 1999)}
\]

Henry’s Law Constant (Pa m^3/mol at 25°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°C, Alaee et al. 1996)

\[
\ln K_{\text{AW}} = 4.6774 - 3235.5/(T/K); \text{ temp range: 5.4–35.3°C (gas stripping-GC, Alaee et al. 1996)}
\]

5.64* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)

\[
\ln K_{\text{AW}} = -5629.06/(T/K) + 12.75, \quad \Delta H = 46.8 \text{ kJ mol}^{-1}, \text{ measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)}
\]

\[
\log [H/(Pa m^3/mol)] = 6.91 - 1363/(T/K), \quad \text{(Passivirta et al. 1999)}
\]

4.58 (20°C, selected from reported experimentally measured data, Staudinger & Roberts 2001)

\[
\log K_{\text{AW}} = 2.065 - 1404/(T/K); \text{ temp range 348–368 K (Knudsen effusion technique, Li et al. 2004)}
\]

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):

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 ± 0.15 (recommended, Sangster 1989, 1993)
4.57 (TLC-RT correlation, De Voogt et al. 1990)
4.45 (recommended, Hansch et al. 1995)
4.53 ± 0.19, 4.55 ± 0.61 (HPLC-k’ correlation: ODS column, Diol column, Helweg et al. 1997)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

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 \( K_{OA} \) at 25°C:
7.30 (calculated-\( K_{ow}/K_{AW} \), Wania & Mackay 1996)
7.34 (calculated, Finizio et al. 1997)
7.55 (calculated-\( S_{oct} \) and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:
3.08, 2.68 (\( \text{Daphnia, pimephales} \), Southworth 1977)
2.88 (\( \text{Daphnia pulex} \), Herbes & Risi 1978)
2.96 (\( \text{Daphnia pulex} \), Southworth et al. 1978)
3.08 (kinetic estimation, Southworth et al. 1978)
3.89 (algae, Geyer et al. 1981)
4.22 (\( \text{P. hoyi} \), 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 (\( \text{Daphnia magna} \), Newsted & Giesy 1987)
0.820, 1.373 (\( \text{Polychaete sp.} \), \( \text{Capitella capitata} \), Bayona et al. 1991)

Sorption Partition Coefficient, log \( K_{OC} \):
4.42 (natural sediment, average of sorption isotherms by batch equilibrium-UV spec., Karickhoff et al. 1979)
3.74 (22°C, suspended particulates, Herbes et al. 1980)
4.20 (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 mg/L DOC, RP-HPLC separation, Landrum et al. 1984)
3.95, 4.73 (humic materials in aqueous solutions: RP-HPLC-LSC, equilibrium dialysis, Lake Erie water with 9.6 mg/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 mg/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 ± 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 exp., Winget et al. 1998)
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 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of ext 1,2,3-solvophobic approach, Krauss & Wilcke 2001)
4.34; 4.26; 3.95–5.70 (calculated-\( K_{ow} \); calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)
4.375 at pH 4, 4.42 at pH 7, 4.39 at pH 10 in 0.001 M NaCl; 4.415 at pH 4, 4.37 at pH 7, 4.30 at pH 10 in 0.01 M NaCl; 4.50 at pH 4, 4.24 at pH 7, 4.27 at pH 10 in 0.1 M NaCl; 4.38 at pH 4, 4.40 at pH 7, 4.12 at pH 10 in 1 mM Ca\textsuperscript{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautman & Morgan 1993a)

4.28 at pH 4, 4.18 at pH 7, 4.20 at pH 10 in 0.001 M NaCl; 4.285 at pH 4, 4.15 at pH 7, 4.22 at pH 10 in 0.01 M NaCl; 4.23 at pH 4, 4.12 at pH 7, 4.20 at pH 10 in 0.1 M NaCl; 4.21 at pH 4, 4.19 at pH 7, 4.24 at pH 10 in 1 mM Ca\textsuperscript{2+} in 0.1 M total ionic strength solutions (shake flask/fluorescence, fulvic acid; Schlautman & Morgan 1993a)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_\text{½}$:

Volatilization: removal rate constants from the water column at 25°C in midsummer sunlight were: $k = 0.002 \text{ h}^{-1}$ in deep, slow, somewhat turbid water; $k = 0.001 \text{ h}^{-1}$ in deep, slow muddy water; $k = 0.002 \text{ h}^{-1}$ in deep slow, clear water; $k = 0.042 \text{ h}^{-1}$ in shallow, fast, clear water; and $k = 0.179 \text{ h}^{-1}$ in very shallow, fast, clear water (Southworth 1977);

aquatic $t_\text{½} = 18–300 \text{ h}$ (Callahan et al. 1979);

calculated $t_\text{½} = 62 \text{ h}$ for a river 1-m deep with water velocity of 0.5 m/s and wind velocity of 1 m/s (Southworth 1979; quoted, Herbes et al. 1980; Hallett & Brecher 1984).

Photolysis: removal rate constants from the water at 25°C in midsummer sunlight were: $k = 0.004 \text{ h}^{-1}$ in deep, slow somewhat turbid water; $k < 0.001 \text{ h}^{-1}$ in deep, slow, muddy water; $k = 0.018 \text{ h}^{-1}$ in deep, slow, clear water; $k = 0.086 \text{ h}^{-1}$ in shallow, fast, clear water; and $k = 0.238 \text{ h}^{-1}$ in very shallow, fast, clear water (Southworth 1977)

24-h photolytic $t_\text{½} \sim 1.6 \text{ h}$ in summer and $t_\text{½} = 4.8 \text{ h}$ in winter at 35°N latitude (Southworth 1977)

direct sunlight $k = 0.15 \text{ h}^{-1}$ in winter at 35°N latitude (Callahan et al. 1979)

t$_\text{½}(\text{calc}) = 0.75 \text{ h}$ near surface water for direct sunlight photolysis at 40°N latitude of midday in midsummer (quoted, Herbes et al. 1980; Harris 1982)

t$_s = 4.5 \text{ d}$ in inland water, and $t_\text{½} = 5.2 \text{ d}$ in inland water with sediment partitioning and $t_\text{½} = 0.75 \text{ h}$ for direct photochemical transformation near surface water (Zepp & Schlotzhauer 1979)

atmospheric and aqueous photolysis $t_\text{½} = 0.58 \text{ h}$, based on measured aqueous photolysis rate constant for midday summer sunlight at 35°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 μg/g on substrate): $t_\text{½} = 2.9 \text{ h}$ on silica gel, $t_\text{½} = 0.5 \text{ h}$ on alumina and $t_\text{½} = 48 \text{ h}$ on flyash (Behymer & Hites 1985)

t$_\text{½} = 4.5 \text{ d}$ for summer at 40°N latitude under sunlight in surface water (Mill & Mabey 1985)

$k = 0.66 \text{ h}^{-1}$ in distilled water with $t_\text{½} = 1.0 \text{ h}$ (Fukuda et al. 1988)

photodegradation $k = 0.023 \text{ min}^{-1}$ and $t_\text{½} = 0.50 \text{ h}$ for initial concentration of 5 ppm in methanol-water (1:1, v/v) solution by high pressure mercury lamp or sunlight (Wang et al. 1991)

pseudo-first-order direct photolysis rate constants, $k(\text{exptl}) = 0.023 \text{ min}^{-1}$ with the calculated $t_\text{½} = 0.50 \text{ h}$, and the predicted $k = 0.030 \text{ min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

$k = 4.7 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant $k$, for gas-phase second order rate constants, $k_{\text{OH}}$ for reaction with OH radical, $k_{\text{NO}_3}$ with NO\textsubscript{3} radical and $k_{\text{O}_3}$ with O\textsubscript{3} or as indicated, *data at other temperatures see reference:

photooxidation $t_\text{½} = 1111–38500 \text{ h}$, based on measured rate constant for reaction with hydroxyl radical in water (Radding et al. 1976; quoted, Howard et al. 1991)

$k(\text{aq})$ rate of 50 L mol\textsuperscript{-1} s\textsuperscript{-1} with $t_\text{½} = 1600 \text{ d}$ (Callahan et al. 1979)

$k(\text{calc}) = 5.0 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$ for singlet O\textsubscript{2} and 2.2 $\times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k(\text{aq}) = 3.3 \times 10^{-4} \text{ s}^{-1}$ with $t_\text{½} = 0.6 \text{ h}$ under natural sunlight conditions (NRCC 1983)

$k_{\text{OH}} = 110 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 325 ± 1 K (relative rate technique for propene, (Biermann et al. 1985; Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 203 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

\[ k = 3.5 \times 10^{-5} \text{ s}^{-1} \], indirect total photoreaction rate constant in surface waters (Mill 1999)

\[ k_{\text{OH}} = 190 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \] at 298 K, measured range 306–366 K with a calculated atmospheric lifetime of 1.5 h based on gas-phase OH reaction (Brubaker & Hites 1998)

Hydrolysis: \( k < 0.001 \text{ h}^{-1} \) at 25°C (Southworth 1977); not hydrolyzable (Mabey et al. 1982); no hydrolyzable groups (Howard et al. 1991).

Biodegradation:

\( k = 0.061 \text{ h}^{-1} \) for microbial degradation in Third Creek water incubated 18 h at 25°C; removal rate constants from water column at 25°C in midsummer sunlight were: \( k = 0.060 \text{ h}^{-1} \) in deep, slow, somewhat turbid water; \( k = 0.030 \text{ h}^{-1} \) in deep, slow, muddy water; \( k = 0.061 \text{ h}^{-1} \) in deep, slow, clear water; \( k = 0.061 \text{ h}^{-1} \) in shallow, fast, clear water; and \( k = 0.061 \text{ h}^{-1} \) in very shallow, fast, clear water (Southworth 1977)

\( k = 0.035 \text{ h}^{-1} \) 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)

\( k = 2.5 \times 10^{-3} \text{ h}^{-1} \) with \( t_{1/2} = 12 \text{ d} \) and \( k = 2.5 \times 10^{-4} \text{ h}^{-1} \) with \( t_{1/2} = 115 \text{ d} \) for mixed bacterial populations in oil-contaminated and pristine stream sediments (Herbes & Schwall 1978, NRCC 1983)

\( t_{1/2} = 1200–11040 \text{ h} \), based on aerobic soil die-away test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991)

\( k = 0.0052 \text{ d}^{-1} \) with \( t_{1/2} = 134 \text{ d} \) for Kidman sandy loam and \( k = 0.0138 \text{ d}^{-1} \) with \( t_{1/2} = 50 \text{ d} \) for McLarin sandy loam all at ~0.33 bar soil moisture (Park et al. 1990)

\( t_{1/2} = 4800–44160 \text{ h} \), based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: aquatic fate rate, \( k < 0.0612 \text{ h}^{-1} \) with \( t_{1/2} > 11.3 \text{ h} \) (Callahan et al. 1979); estimated rate constant for bacteria of \( 3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1} \) (Mabey et al. 1982).

Biocemdration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

log \( k_1 = 2.89 \text{ h}^{-1} \); log \( k_2 = 0.0043 \text{ h}^{-1} \) (Daphnia pulex, Herbes & Risi 1978)

\( k_1 = 702 \text{ h}^{-1} \); \( k_2 = 0.589 \text{ h}^{-1} \) (Daphnia pulex, Southworth et al. 1978)

\( k_1 = (1.73 \times 10^{-3} – 36) \text{ h}^{-1} \); \( k_2 = 0.040 \text{ h}^{-1} \) (average, bluegill sunfish, Spacie et al. 1983)

log \( k_1 = 2.85 \text{ h}^{-1} \); log \( k_2 = -0.23 \text{ h}^{-1} \) (Daphnia pulex, correlated to Mackay & Hughes 1984, Hawker & Connell 1986)

\( k_1 = 1.46, 16.9 \text{ h}^{-1} \); \( k_2 = (1.58–1.88) \times 10^{-3} \text{ h}^{-1} \) (rainbow trout, Linder et al. 1985)

\( k_1 = 87.2 \text{ h}^{-1} \); \( k_2 = 0.019 \text{ h}^{-1} \) (4°C, S. heringianus, Frank et al. 1986)

\( k_1 = 131.1 \text{ mL g}^{-1} \text{ h}^{-1} \); \( k_2 = 0.0033 \text{ h}^{-1} \) (4°C, P. hoyi, Landrum 1988)

log \( k_1 = 2.2, -0.01 \text{ d}^{-1} \) (fish, calculated-K_{OW}, Thomann 1989)

log \( k_2 = -0.96 \text{ d}^{-1} \) (oyster, calculated-K_{OW}, Thomann 1989)

\( k_1 = 1.8–2.3 \text{ mg g}^{-1} \text{ h}^{-1} \); \( k_2 = 0.045 \text{ h}^{-1} \) (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: \( t_{1/2} = 0.58–1.7 \text{ h} \), based on photolysis half-life in water (Howard et al. 1991);

-half-lives under simulated atmospheric conditions: \( t_{1/2} = 0.20 \text{ h} \) for simulated sunlight, \( t_{1/2} = 0.15 \text{ h} \) for simulated sunlight + ozone with concn of 0.2 ppm, \( t_{1/2} = 1.23 \text{ h} \) 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°C in midsummer sunlight were, \( t_{1/2} = 10.5 \text{ h} \) for deep, slow, somewhat turbid water; \( t_{1/2} = 21.6 \text{ h} \) for deep, slow, muddy water; \( t_{1/2} = 8.5 \text{ h} \) for deep, slow, clear water; \( t_{1/2} = 3.5 \text{ h} \) for shallow, fast, clear water; and \( t_{1/2} = 1.4 \text{ h} \) for very shallow, fast, clear water (Southworth 1977, Herbes et al. 1980);

computed near-surface \( t_{1/2} = 0.75 \text{ h} \) of a water body and for direct photochemical transformation at latitude 40°N, midday, midsummer and half-lives: \( t_{1/2} = 4.5 \text{ d} \) for no sediment-water partitioning, \( t_{1/2} = 5.2 \text{ d} \) with sediment-water partitioning and for direct photolysis in a 5-m deep inland water body (Zepp & Schlotzhauer 1979);

\( t_{1/2} = 0.58–1.7 \text{ h} \), based on photolysis half-life in water (Howard et al. 1991);

\( t_{1/2} = 4.5 \text{ d} \) at 40°N under summer sunlight (Mill & Mabey 1985);

photolysis \( t_{1/2} = 0.50 \text{ h} \) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996);

indirect photoreaction \( t_{1/2} = 5.5 \text{ h} \) in surface waters (Mill 1999);
photolysis $t_{1/2} = 13.3$–$13.80$ min at $15^\circ$C in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater: $t_{1/2} =$ 2400–22080 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction $t_{1/2} =$ 600 h for chemical available anthracene and $t_{1/2} =$ 77 h for bioavailable anthracene for amphipod, $P$. hoi in Lake Michigan sediments at $4^\circ$C. The uptake clearance from sediment was $(0.024 \pm 0.002)g$ of dry sediment·g$^{-1}$ of organism·h$^{-1}$, and the rate constants to become biologically unavailable were $(0.009 \pm 0.002)h^{-1}$ corresponding to $t_{1/2} =$ 77 h (Landrum 1989).

Soil: $t_{1/2} =$ 3.3 – 175 d (Sims & Overcash 1983; quoted, Bulman et al. 1987);
$\quad t_{1/2} =$ 17 d for 5 mg/kg treatment and $t_{1/2} =$ 45 d for 50 mg/kg treatment (Bulman et al. 1987);
$\quad$ degradation rate constant $k =$ 0.0052 d$^{-1}$ with $t_{1/2} =$ 134 d for Kidman sandy loam soil and $k =$ 0.138 d$^{-1}$ with $t_{1/2} =$ 50 d for McLauren sandy loam soil (Park et al. 1990);
$\quad t_{1/2} =$ 1200–11040 h, based on aerobic soil die-away test data (Howard et al. 1991);
$\quad t_{1/2} =$ 0.5–26 wk, 7.9 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: $t_{1/2} =$ 17 h in bluegill sunfish (Spacie et al. 1983); with depuration $t_{1/2} =$ 37.75 h in $s$. heringianus (Frank et al. 1986); elimination $t_{1/2} =$ 7 d from rainbow trout, $t_{1/2} =$ 1.9 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

$$R \cdot \ln x = \frac{\Delta H_{fus}}{(T/K)} + (0.000408)\left(\frac{(T/K) – 291.15}{2} – c + b \cdot (T/K)\right)$$  \hspace{1cm} (1)

$$\frac{S}{(\mu g/kg)} = a \cdot t^3 + b \cdot t^2 + c \cdot t + d$$ \hspace{1cm} (2)

$$\ln x = A – B/T(K)$$ \hspace{1cm} (3)

$$\ln x = A + B/(T/K) + C \cdot \ln (T/K)$$ \hspace{1cm} (4)

$$\ln x = A + \frac{B}{\tau} + C \cdot \ln \tau,$$ \hspace{1cm} \text{where } \tau = T/T_0, \quad T_0 = 298.15K \hspace{1cm} (4a)

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<th>$t/°C$</th>
<th>$S/\text{g·m}^{-3}$</th>
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$\Delta H_{sol}$/$(kJ \text{ mol}^{-1}) = 34.81$
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(Continued)
**TABLE 4.1.1.25.1 (Continued)**

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*tentative

$\Delta H_{sol}/(kJ \text{ mol}^{-1}) = 45.2 ± 0.3$ at 298.15 K.

$\Delta H_{sol}/(kJ \text{ mol}^{-1}) = 29.37$

**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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C\cdot\log(T/K) \quad (4)
\end{align*}
\]

1. **Nelson & Senseman 1922**
   - isoteniscope-Hg manometer

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bp/°C: 342 (temp range 232–340°C)

**Mortimer & Murphy 1923**
   - isoteniscope-Hg manometer

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**Stull 1947**
   - summary of literature data

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**Rodebush gauge**
   - measured range 105–125°C

\[ \Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 97.70 \]

2. **Bradley & Cleasby 1953**
   - effusion

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bp/°C: 342 (temp range 232–340°C)

**Kelley & Rice 1964**
   - effusion

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**Malaspina et al. 1973**
   - Knudsen effusion

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>79.55</td>
<td>0.612</td>
</tr>
<tr>
<td>88.25</td>
<td>1.373</td>
</tr>
<tr>
<td>98.05</td>
<td>3.506</td>
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</table>

**Power et al. 1977**
   - gas saturation

<table>
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<tr>
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(Continued)
### TABLE 4.1.125.2 (Continued)

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<tr>
<td>B 5320</td>
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<td></td>
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<td>105 3.880</td>
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<tr>
<td>A 11.638</td>
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<td></td>
<td>12.3 1.64 × 10⁻⁴</td>
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<tr>
<td>B 5320</td>
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<td>12.3 1.57 × 10⁻⁴</td>
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<tr>
<td>86.65</td>
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<td>eq. 1 P/mmHg</td>
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<td>A 12.616</td>
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<td>30.1 1.46 × 10⁻³</td>
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<td></td>
<td></td>
<td>34.93 2.59 × 10⁻³</td>
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</tr>
<tr>
<td>34.93 2.63 × 10⁻³</td>
<td></td>
<td></td>
<td></td>
<td>34.93 2.69 × 10⁻³</td>
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<td>B 4891.87</td>
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<td>$t/^{\circ}C$</td>
<td>$P/Pa$</td>
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<td>4.99</td>
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<td>21.30</td>
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<tr>
<td>B</td>
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<td>139.7</td>
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<tr>
<td>$\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 98.79$</td>
<td>$\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 102.6$</td>
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**FIGURE 4.1.1.25.2** Logarithm of vapor pressure versus reciprocal temperature for anthracene.

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### TABLE 4.1.1.25.3
Reported Henry’s law constants of anthracene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>H/(Pa·m³/mol)</th>
<th>H/(Pa·m³/mol)</th>
<th>H/(Pa·m³/mol)</th>
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</thead>
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<td>5.4</td>
<td>2.76</td>
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<td>1.14, 1.38</td>
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<td>3.12</td>
<td>11.0</td>
<td>1.99, 2.26</td>
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<td>14.8</td>
<td>3.44</td>
<td>18.0</td>
<td>3.31, 3.70</td>
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<td>20.6</td>
<td>3.91</td>
<td>25.0</td>
<td>5.26, 6.06</td>
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<td>25.0</td>
<td>4.94</td>
<td>31.0</td>
<td>7.60, 9.18</td>
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<td>8.05</td>
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</tr>
<tr>
<td>34.3</td>
<td>8.94</td>
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<td></td>
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**Average**

<table>
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<th>Temperature (°C)</th>
<th>H/(Pa·m³/mol)</th>
<th>H/(atm·m³/mol)</th>
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</thead>
<tbody>
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<td>25.0</td>
<td>4.94</td>
<td>8.36</td>
</tr>
</tbody>
</table>

### Alae et al. 1996

- **Gas stripping-GC**
  - \(K_{AW} = A - B·(T/K) + C·(T/K)^2\) (5)

### Bamford et al. 1999

- **Gas stripping-GC/MS**
  - Equation 1: \(\ln K_{AW} = A - B/(T/K)\) (1)
  - \(\log K_{AW} = A - B/(T/K)\) (1a)
  - \(\ln (1/K_{AW}) = A - B/(T/K)\) (2)
  - \(\log (1/K_{AW}) = A - B/(T/K)\) (2a)
  - \(\ln [H/(Pa·m³/mol)] = A - B/(T/K)\) (4)
  - \(\ln [H/(atm·m³/mol)] = A - B/(T/K)\) (4a)
  - \(K_{AW} = A - B·(T/K) + C·(T/K)^2\) (5)

#### Enthalpy and Entropy Change

- **ΔH/(kJ·mol⁻¹)** = 46.8 ± 1.7
- **ΔS/(J·K⁻¹·mol⁻¹)** = 106

#### Enthalpy of Volatilization

- **ΔHvol/(kJ·mol⁻¹)** = 26.9 at 25°C

---

**FIGURE 4.1.1.25.3** Logarithm of Henry’s law constant versus reciprocal temperature for anthracene.
4.1.1.26 2-Methylnaphthacene

Common Name: 2-Methylnaphthacene
Synonym:
Chemical Name: 2-methylnaphthacene
CAS Registry No: 613-12-7
Molecular Formula: C_{15}H_{12}
Molecular Weight: 192.256
Melting Point (°C):
209 (Weast 1982–83; Lide 2003)
Boiling Point (°C):
359 (sublimation, Bjørseth 1983)
Density (g/cm³ at 20°C):
1.80 (0°C, Lide 2003)
Molar Volume (cm³/mol):
106 (calculated-density, liquid molar volume, Lande & Banerjee 1981)
218.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0157 (mp at 209°C)
Water Solubility (g/m³ or mg/L at 25°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°C, May et al. 1978a)
0.0213 (generator column-HPLC/UV, measured range 5–30°C, May et al. 1978b)
S/(µg/kg) = 324.0 + 5.413·(t/°) + 0.8059·(t/°C)² + 0.0025·(t/°C)³; temp range 5–30°C (generator column-HPLC/UC, May et al. 1978b)
0.0191* (23.1°C, generator column-HPLC/fluor., temp range 278.25–302.45 K, May et al. 1983)
0.031 (average lit. value, Pearlman et al. 1984)
0.0225* (generator column-HPLC/UV, measured range 4.6–25.3°C, Whitehouse 1984)
0.03* (tentative value, IUPAC Solubility Data Series, Shaw 1989)
ln x = –1.841995 – 4616.86/(T/K), temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
0.0262* (generator column-HPLC/UV, measured range 0–50°C, Dohányosová et al. 2003)
ln x = –42.7975 + 22.9752/τ + C ln τ, τ = T/298.15 K; temp range 0–50°C (generator column-HPLC/UV, Dohányosová et al. 2003)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.0207 (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)
log (P_L/Pa) = –3976/(T/K) + 11.65; ΔH_{vap} = –76.1 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow} at 25°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)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:
- Volatilization:
- Photolysis:
- Hydrolysis:
- Oxidation:

Half-Lives in the Environment:
- Biota: elimination $t_{1/2} = 2$ 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

\[
S/(\mu g/kg) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)
\]
\[
\ln \, x = A + B/\tau + C \ln \tau \quad (2)
\]

where $\tau = T/T_o$ and $T_o = 298.15 \, K$

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<tr>
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<tr>
<td>generator column-HPLC</td>
<td>generator column-HPLC/UV</td>
<td>IUPAC “tentative” values</td>
<td>generator column-HPLC</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
<td>t/°C</td>
<td>S/g·m⁻³</td>
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<tr>
<td>6.3</td>
<td>0.00706</td>
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<td>–</td>
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<tr>
<td>9.1</td>
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<td>13.9</td>
<td>0.0111</td>
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<td>18.3</td>
<td>0.0145</td>
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<td>23.1</td>
<td>0.0191</td>
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<td>27.0</td>
<td>0.0242</td>
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<td>0.0321</td>
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</tbody>
</table>

Temp dependence eq. 1

\[ S/\mu g/kg = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \]

\[ \ln \, x = A + B/\tau + C \ln \tau \]

where $\tau = T/T_o$ and $T_o = 298.15 \, K$

\[ \Delta H_{sol}/(kJ \cdot mol⁻¹) = 39.08 \]

\[ \Delta H_{sol}/(kJ \cdot mol⁻¹) = 46.15 \pm 0.3 \, 0.3 \] at 298.15 K

\[ \Delta H_{mp}/K = 479 \]

\[ \Delta H_{sol}/(kJ \cdot mol⁻¹) = 24.06 \]
FIGURE 4.1.1.26.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-methylanthracene.
4.1.1.27 9-Methylandranthracene

Common Name: 9-Methylandranthracene
Synonym:
Chemical Name: 9-methylandranthracene
CAS Registry No: 779-02-2
Molecular Formula: C_{15}H_{12}
Molecular Weight: 192.256
Melting Point (°C):
81.5  (Weast 1982–83; Lide 2003)
Boiling Point (°C):
196  (12 mm Hg, Weast 1982–83; Lide 2003)
Density (g/cm³ at 20°C):
1.065  (99°C, Lide 2003)
Molar Volume (cm³/mol):
181  (calculated-density, liquid molar volume, Lande & Banerjee 1981)
218.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.279 (mp at 81.5°C)

Water Solubility (g/m³ or mg/L at 25°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°C, Dohányosová et al. 2003)
ln x = –76.9798 + 59.8386/τ + C  ln τ, τ = T/298.15 K, temp range 0–50°C (generator column-HPLC/UV, Dohányosová et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
0.00224  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_L/kPa) = 11.683 – 5168/(T/K); temp range 354–402 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
5.12  (calculated-π 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 ± 0.20  (recommended, Sangster 1989, 1993)
5.07  (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:
3.66; 3.59  (Daphnia pulex; kinetic estimation, Southworth et al. 1978)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

3.75 (calculated-$K_{ow}$, Mackay 1982)
3.94 (calculated-MCI $\chi$, Sabljic 1987b)
3.683, 3.778 (calculated-MCI $\chi$, calculated-$K_{ow}$, Lu et al. 1999)

Sorption Partition Coefficient, log $K_{OC}$:
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 $\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, $k$, or Half-Lives, $t_1/2$:
Volatilization:
Photolysis:
\[ t_{1/2}(calc) = 0.13 \text{ h} \text{ for direct photochemical transformation near water surface and } t_{1/2} = 0.78 \text{ d} \text{ for no sediment-water partitioning; and } t_{1/2} = 1.2 \text{ d} \text{ with sediment-water partitioning (Zepp & Scholtzhauer 1979)} \]
\[ t_{1/2} = 0.79 \text{ d} \text{ for summer at 40°N latitude under sunlight in surface water (Mill & Mabey 1985)} \]
photodegradation $k = 0.163 \text{ min}^{-1}$ and $t_{1/2} = 0.07 \text{ h}$ in methanol-water (2:3, v/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 $k(\text{exp}) = 0.0163 \text{ min}^{-1}$ with calculated $t_{1/2} = 0.07 \text{ h}$ and the predicted $k(\text{calc}) = 0.00343 \text{ min}^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
direct photolysis $t_{1/2} = 1.85 \text{ h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
Oxidation: $t_{1/2} = 10 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:
Biodegradation:
Biotransformation:
Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:
\[ k_1 = 561 \text{ h}^{-1}; k_2 = 0.144 \text{ h}^{-1} \text{ (Daphnia pulex, Southworth et al. 1978)} \]
\[ \log k_1 = 2.75 \text{ h}^{-1}; \log k_2 = -0.84 \text{ h}^{-1} \text{ (Daphnia pulex, correlated as per Mackay & Highes 1984, Hawker & Connell 1986)} \]

Half-Lives in the Environment:
Air: direct photolysis $t_{1/2} = 1.85 \text{ h}$ predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
Surface water: computed $t_{1/2} = 0.13 \text{ h}$ at near-surface of a water body, for direct photochemical transformation, and $t_{1/2} = 0.79 \text{ d}$ for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning, $t_{1/2} = 1.2 \text{ d}$ with sediment-water partitioning to top cm bottom sediment; and $t_{1/2} = 10 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979);
\[ t_{1/2} = 0.79 \text{ d} \text{ for summer at 40°N latitude under sunlight (Mill & Mabey 1985)} \];
photolysis $t_{1/2} = 0.07 \text{ h}$ in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater:
Sediment:
Soil:
Biota: elimination $t_{1/2} = 4 \text{ d}$ 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

\[ \ln x = A + B/\tau + C \ln \tau, \text{ where } \tau = T/T_o \text{ and } T_o = 298.15 \text{ K} \quad (1) \]

Dohányosová et al. 2003

<table>
<thead>
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<th>t/°C</th>
<th>S/g·m(^{-3})</th>
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</tbody>
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eq 1 mole fraction
A –76.9798
B 59.8386
C 76.7066

\[ \Delta H_{\text{sol}}/(kJ \text{ mol}^{-1}) = 41.8 \pm 0.2 \quad \text{at 298.15 K} \]

\[ \Delta H_{\text{fus}}/(kJ \text{ mol}^{-1}) = 16.95 \]

FIGURE 4.1.1.27.1 Logarithm of mole fraction solubility (\(\ln x\)) versus reciprocal temperature for 9-methylanthracene.
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: C_{16}H_{14}
Molecular Weight: 206.282
Melting Point (°C):
183.6 (Lide 2003)
Boiling Point (°C):
360 (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
241.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0278 (at mp = 183.6°C)

Water Solubility (g/m³ or mg/L at 25°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°C, Dohányosová et al. 2003)
ln x = –73.2594 + 52.6685/τ + C ln τ, τ = T/298.15 K; temp range 0–50°C (generator column-HPLC/UV, Dohányosová et al. 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
1.53 × 10⁻⁴ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_s/kPa) = 11.266 – 5391/(T/K); temp range 381–434 K (Antoine eq., Stephenson & Malanowski 1987)

Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{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 K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k or Half-Lives, t_½:
Volutilization:
Photolysis: direct photochemical transformation t_½(calc) = 0.35 h, computed near-surface water, latitude 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)
photodegradation in methanol-water (2:3, v/v) solution for initial concentration of 5 ppm by high pressure mercury lamp or sunlight with a rate constant k = 0.0633 min⁻¹ and t_½ = 0.18 h (Wang et al. 1991)
pseudo-first-order direct photolysis $k_{\text{exptl}} = 0.0633 \text{ min}^{-1}$ with the calculated $t_{1/2} = 0.18 \text{ h}$ and the predicted $k_{\text{calc}} = 0.0379 \text{ min}^{-1}$ calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

direct photolysis $t_{1/2} = 1.17 \text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Oxidation: $t_{1/2} = 1.5 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 1.17 \text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis $t_{1/2} = 0.35 \text{ h}$ near surface water, 40°N; midday, midsummer and photosensitized oxygenation $t_{1/2} = 1.5 \text{ h}$ at near surface water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979).

photolysis $t_{1/2} = 0.18 \text{ h}$ 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

\[
\ln x = A + \frac{B}{\tau} + C \ln \tau, \text{ where } \tau = T/T_o \text{ and } T_o = 298.15 \text{ K} \quad (1)
\]

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generator column-HPLC

<table>
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<th>t/°C</th>
<th>S/g·m⁻³</th>
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<tbody>
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<td>0.000391</td>
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<tr>
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</tr>
<tr>
<td>50</td>
<td>0.0728</td>
</tr>
</tbody>
</table>

eq. 1 mole fraction

A = -73.2594

B = 52.6685

C = 71.9873

\[\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 47.9 \pm 0.3\]

at 298.15 K

mp/K = 455

\[\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.46\]
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: \( \text{C}_{16}\text{H}_{10} \)
Molecular Weight: 202.250
Melting Point (°C):
\[ 150.62 \text{ (Lide 2003)} \]
Boiling Point (°C):
\[ 404 \text{ (Lide 2003)} \]
Density (g/cm³ at 20°C):
\[ 1.271 \text{ (23°C, Weast 1982–83; Lide 2003)} \]
Molar Volume (cm³/mol):
\[ 159.0 \text{ (calculated-density, liquid molar volume, Lande & Banerjee 1981)} \]
\[ 213.8 \text{ (calculated-Le Bas method at normal boiling point)} \]
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
\[ 17.11 \text{ (Ruelle & Kesselring 1997)} \]
\[ 0.29, 17.36; 17.65 \text{ (–152.35, 150.65°C; total phase change enthalpy, Chickos et al. 1999)} \]
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
\[ 35.98 \text{ (Wauchope & Getzen 1972)} \]
\[ 40.17 \text{ (Casellato et al. 1973)} \]
\[ 54.8 \text{ (Hinckley et al. 1990)} \]
\[ 40.97 \text{ (150.65°C, Chickos et al. 1999)} \]
\[ 43.36, 43.8 \text{ (exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)} \]
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \text{ J/mol K} \)), \( F \):
\[ 0.0585 \text{ (mp at 150.62°C)} \]
\[ 0.128 \text{ (calculated, \( \Delta S_{\text{ fus}} = 40.3 \text{ J/mol K} \), Passivirta et al. 1999)} \]
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
\[ 0.165 \text{ (27°C, shake flask-nephelometry, Davis et al. 1942)} \]
\[ 0.175 \text{ (shake flask-UV, Klevens 1950)} \]
\[ 0.148 \text{ (Pierotti et al. 1959)} \]
\[ 1.56 \text{ (shake flask-UV/fluorescence, Barone et al. 1967)} \]
\[ 0.105 \text{ (20°C, shake flask-UV, Eisenbrand & Baumann 1970)} \]
\[ 0.148* \text{ (shake flask-UV, measured range 22.2–74.7°C, Wauchope & Getzen 1972)} \]
\[ R \ln x = −3660/(T/K) + 4.08 \times 10^{-4} \cdot (T/K) − 291.15 \cdot (T/K)^2 − 38.1 + 0.0478 \cdot (T/K); \text{ temp range 22.2–73.4°C (shake flask-UV measurements, Wauchope & Getzen 1972)} \]
\[ 0.105, 0.133, 0.107, 0.069 \text{ (HPLC-relative retention correlation, different stationary and mobile phases, Locke 1974)} \]
\[ 0.171 \text{ (shake flask-fluorescence/UV, Schwarz & Wasik 1976)} \]
\[ 0.135 \text{ (shake flask-fluorescence, Mackay & Shiu 1977)} \]
\[ 0.132 \text{ (Rossi 1977; Neff 1979)} \]
\[ 0.1295* \text{ (shake flask-fluorescence, measured range 12.2–31.3°C, Schwarz 1977)} \]
\[ 0.132* \text{ (generator column-HPLC/UV, measured range 5–30°C, May et al. 1978b)} \]
\[ S/(\mu g/\text{kg}) = 50.2 − 1.051 \cdot (t/°C) + 0.2007 \cdot (t/°C)^2 − 0.0011 \cdot (t/°C)^3; \text{ temp range 5–30°C (generator column-HPLC/UV, May et al. 1978b)} \]
\[ 0.032 \text{ (shake flask-nephelometry, Hollifield 1979)} \]
\[ 0.135 \text{ (shake flask-LSC, Means et al. 1979; 1980)} \]
\[ 0.130 \text{ (shake flask-VC/UV, Rossi & Thomas 1981)} \]
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

0.136* (25.5°C, 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 (solid SS at 26°C); 2.61, 1.01 (supercooled liquid S_L at 4°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)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00339 (effusion method, Inokuchi et al. 1952)
0.000882* (effusion method, extrapolated from Antoine eq., Bradley & Cleasby 1953)
\[ \log (P/cmHg) = 10.270 - 4904/(T/K); \text{ temp range 71.75–85.25°C (Antoine eq., Bradley & Cleasby 1953)} \]
347* (200.4°C, temp range 200.4–394.7°C, Tsypkina 1955; quoted, Boublik et al. 1984)
0.00033 (effusion method, Hoyer & Peperle 1958; quoted, Mabey et al. 1982; Tsai et al. 1991)
\[ \log (P/mmHg) = 12.0 - 5248/(T/K); \text{ temp range 25–90°C, (Knudsen effusion method, Hoyer & Peperle 1958)} \]
0.2118* (348 K, Knudsen effusion, measured range 348–419 K, Malaspina et al. 1974)
12.4* (125°C, inclined-piston gauge, measured range 125–185°C, Smith et al. 1980)
0.00091 (effusion method, Pupp et al. 1974; quoted, Bidleman 1984)
0.000871 (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 (P/kPa) = 12.748 – 4760.73/(T/K); temp range 10–50°C (solid, Antoine eq., Sonnefeld et al. 1983)
0.0006 (generator column-HPLC/fluo./UV, Wasik et al. 1983)
0.0113, 0.0049 (P_G by GC-RT correlation with eicosane as reference standard, different GC columns, Bidleman 1984)
0.0158 (supercooled liquid P_L, converted from literature P_S with S_fus Bidleman 1984)
\[ \log (P_L/kPa) = 4.75092 – 1127.529/(16.02 + t°C); \text{ temp range 200–394°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)} \]
0.00442 (Yamasaki et al. 1984)
\[ \log (P_L/mmHg) = 5.6184 – 1122.0/(15.2 + t°C); \text{ temp range 200–395°C (Antoine eq., Dean 1985, 1992)} \]
0.00033 (selected, Howard et al. 1986; quoted, Banerjee et al. 1990)
0.00055 (interpolated Antoine eq.-I, Stephenson & Malanowski 1987)
\[ \log (P_S/kPa) = 10.75452 – 5072.78/(T/K); \text{ temp range 298–401 K (Antoine eq.-I, Stephenson & Malanowski 1987)} \]
\[ \log (P_L/kPa) = 11.35032 – 5286.784/(T/K); \text{ temp range 360–419 K (Antoine eq.-II, Stephenson & Malanowski 1987)} \]
\[ \log (P_L/kPa) = 5.5106 – 1743.57/(-170.83 + T/K), \text{ temp range 513–668 K, (Antoine eq.-III, Stephenson & Malanowski 1987)} \]
0.000413, 0.00973 (lit. mean, supercooled liquid value P_L, Bidleman & Foreman 1987)
0.000293* (pressure gauge, extrapolated-Antoine eq. derived exptl. data, temp 80–140°C, Sasse et al. 1988)
\[ \log (P_L/mmHg) = 8.654859 – 2967.129/(182.314 + t°C); \text{ temp range 80.11–139.97°C (solid, Antoine eq., pressure gauge, Sasse et al. 1988)} \]
\[ \log (P_L/mmHg) = 5.62672 – 1553.755/(112.964 + t°C); \text{ temp range 139.93–194.16°C (liquid, Antoine eq., pressure gauge, Sasse et al. 1988)} \]
0.010, 0.014 (quoted P\textsubscript{L}, supercooled liquid P\textsubscript{L}, GC-RT correlation, Hinckley 1989)
0.0158, 0.0144 (supercooled P\textsubscript{L}, converted from literature P\textsubscript{S} with different $\Delta S_{\text{fus}}$ values, Hinckley et al. 1990)
0.0113, 0.00752 (P\textsubscript{GC} by GC-RT correlation with different reference standards, Hinckley et al. 1990)

$$\log\left(\frac{P}{\text{Pa}}\right) = 11.92 - 4104/(T/K)$$ (GC-RT correlation, Hinckley et al. 1990)

log (P/mmHg) = 70.7671 – 6.9413 × 10^{-3}/(T/K) + 1.5767 × 10^{-12}/(T/K)^2; temp range 424–926 K (vapor pressure eq., Yaws 1994)

0.000446 (supercooled liquid P\textsubscript{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°C, Oja & Suuberg 1998)

$$\log\left(\frac{P}{\text{Pa}}\right) = 33.856 - 12400/(T/K);$$ temp range 308–398 K (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)

Henry's Law Constant (Pa m\textsuperscript{3}/mol 25°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 (gas stripping, Mackay & Shiu 1981)
1.21 (gas stripping-fluorescence, Shiu & Mackay 1997)
2.0, 0.92 (gas stripping-HPLC/fluorescence, De Maagd et al. 1998)
0.496 (wetted wall column-GC, Altschuh et al. 1999)

$$\ln K_{\text{AW}} = -5159.97/(T/K) + 10.103, \Delta H = 42.9 \text{ kJ mol}^{-1},$$ measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

log [H/(Pa m\textsuperscript{3}/mol)] = 9.17 – 2475/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:

4.90 (calculated-π 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-k' 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 ± 0.20 (recommended, Sangster 1989, 1993)
4.88 (recommended, Hansch et al. 1995)
5.08; 5.39 (26°C; 4°C, Piatt et al. 1996)
4.84 ± 0.19, 5.14 ± 0.62 (HPLC-k' correlation: ODS column; Diol column, Helweg et al. 1997)
4.77 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schrädé 1999)
4.79 (shake flask-SPME solid-phase micro-extraction, Paschke et al. 1999)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°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-$K_{OW}/K_{AW}$, Wania & Mackay 1996)
8.61  (calculated, Finizio et al. 1997)
8.80*; 8.49  (generator column-GC; calculated-$C_{p}/C_{A}$, measured range 0–40°C, Harner & Bidleman 1998)
log $K_{OA}$ = –4.56 + 3985/(T/K); temp range 0–40°C (generator column-GC, Harner & Bidleman 1998)
8.75  (calculated-$S_{oct}$ and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

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, Selenastrum 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  ($Polychaete$, Shrimo-hepatopancreas, Gobas & Mackay 1989)
0.716, 1.124  ($Polychaete sp$, Capitella capitata, Bayona et al. 1991)

Sorption Partition Coefficient, log $K_{OC}$:

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-$K_{OW}$ regess of $K_{p}$ 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 cm; Spectacle Island 14–16 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 cm, Chin & Gschwend 1992)
4.78; 4.78, 4.78 (sediment: concn ratio $C_{sed}/C_{w}$, concn-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) (4°C, low organic carbon sediment $f_{OC} = 0.0002$, batch equilibrium; column expl., Piatt et al. 1996)
4.62 (range 4.56–4.67); 4.0 (range 3.98–4.00) (26°C, low organic carbon sediment f_{OC} = 0.0002, batch equilibrium; column exptl., Piatt et al. 1996)
4.42–2.56 (5 soils, 20°C, batch equilibrium-sorption isotherm measured by HPLC/UV, Bayard et al. 1998)
5.14, 5.22, 5.23, 5.12, 5.24, 5.45; mean 4.98 ± 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 ± 0.056 (HPLC-screening method with different LC-columns, Szabo et al. 1999)
4.66, 4.70, 4.53 (calculated-K_{ow}; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)
4.50 at pH 4, 4.37 at pH 7, 4.33 at pH 10 in 0.001M NaCl; 4.35 at pH 4, 4.20 at pH 7, 4.245 at pH 10 in 0.01M NaCl; 4.35 at pH 4, 4.15 at pH 7, 4.15 at pH 10 in 0.1M NaCl; 4.29 at pH 7, 4.15 at pH 10 in 1mM Ca^{2+} in 0.1M total ionic strength solutions (shake flask/fluorescence, humic acid; Schlautmam & Morgan 1993a)
4.19 at pH 4, 3.89 at pH 7, 3.92 at pH 10 in 0.001M NaCl; 4.15 at pH 4, 3.88 at pH 7, 3.86 at pH 10 in 0.01M NaCl; 4.08 at pH 4, 3.81 at pH 7, 3.785 at pH 10 in 0.1M NaCl; 4.08 at pH 4, 3.90 at pH 7, 4.06 at pH 10 in 10M Ca^{2+} in 0.1M 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 technique-HPLC/fluorescence, ten Hu lscher et al. 2003)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:
Volatileization: sublimation rate constant of 1.1 × 10^{-4} s^{-1} was measured as loss from glass surface at 24°C at an air flow rate of 3 L/min (Cope & Kalkwarf 1987)
Photolysis: calculated t_{1/2} = 4.2 d for direct sunlight photolysis in midday of midsummer at 40°N for inland water, and t_{1/2} = 5.9 d for inland water with sediment partitioning (Zepp & Schlotzhauer 1979)
\[ k = 1.014 \text{ h}^{-1} \] (Zepp 1980)
\[ t_{1/2} = 0.68 \text{ hm atmospheric and aqueous photolysis half-life, based on measured aqueous photolysis quantum yields calculated for midday summer sunlight at 40°N latitude (Zepp & Schlotzhauer 1979; quoted, Harris 1982; Howard et al. 1991)} \]
\[ t_{1/2} = 2.04 \text{ h after adjusting for approximate winter sunlight intensity (Lyman et al. 1982; quoted, Howard et al. 1991)} \]
\[ t_{1/2} = 31 \text{ h on silica gel, } t_{1/2} = 31 \text{ h on alumina and } t_{1/2} = 46 \text{ h on fly ash on different atmospheric particulate substrates (approximate 25 μg/g on substrate) (Behymer & Hites 1985)} \]
\[ t_{1/2} = 4.2 \text{ d for summer sunlight photolysis in surface water (Mill & Mabey 1995)} \]
\[ k < 1.05 \times 10^{-4} \text{ m/s at 24°C with } [O_3] = 0.16 \text{ ppm and light intensity of 1.3 kW/m² on glass surface of(Cope & Kalkwarf 1987)} \]
photodegradation \[ t_{1/2} = 1 \text{ h in summer to days in winter by sunlight for adsorption on airborne particulates (Valerio et al. 1991)} \]
photolysis \[ t_{1/2} = 0.68 \text{ h in water, based on direct photolysis in sunlight at midday, midsummer, latitude 40°N (Zepp 1991)} \]
\[ k(\text{exptl}) = 0.00362 \text{ min}^{-1} \text{ for pseudo-first-order direct photolysis, with } t_{1/2} = 3.18 \text{ h, and the predicted } k(\text{calc}) = 0.00382 \text{ min}^{-1} \text{ by QSQR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)} \]
\[ t_{1/2}(\text{obs.}) = 2.63 \text{ h, } t_{1/2}(\text{calc}) = 2.56 \text{ h by QSQR in atmospheric aerosol (Chen et al. 2001)} \]
\[ k = (2.08 \pm 0.13) \times 10^{-5} \text{ s}^{-1} \text{ and } t_{1/2} = (9.24 \pm 0.53) \text{h in diesel particulate matter, photochemical degradation under atmospheric conditions, } k = (1.88 \pm 0.16) \times 10^{-5} \text{ s}^{-1} \text{ and } t_{1/2} = (10.22 \pm 0.95) \text{h in diesel particulate matter/sand mixture, and } t_{1/2} = 0.80 \text{ to 1.59 h in various soil components using a 900-W photo-irradiator as light source; } k = (2.61 \pm 0.53) \times 10^{-7} \text{ s}^{-1} \text{ and } t_{1/2} = (737.55 \pm 124.49) \text{h in diesel particulate matter using a 300 W light source (Matsuzawa et al. 2001)} \]
Photodegradation \( k = 3.9 \times 10^{-4} \, \text{s}^{-1} \) in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant \( k \), for gas-phase second order rate constants, \( k_{\text{OH}} \) for reaction with OH radical, \( k_{\text{NO}_3} \) with \( \text{NO}_3 \) radical and \( k_{\text{O}_3} \) with \( \text{O}_3 \) as indicated, *data at other temperatures see reference:

\[ k = 5 \times 10^8 \, \text{M}^{-1} \, \text{h}^{-1} \] for singlet oxygen and \( 2.2 \times 10^4 \, \text{M}^{-1} \, \text{h}^{-1} \) for peroxy radical (Mabey et al. 1982)

\[ k = (3.4–5.3) \times 10^4 \, \text{dm}^3 \, \text{mol}^{-1} \, \text{s}^{-1} \] over pH range 1–7, with \( t_{\frac{1}{2}} = 0.18 \, \text{s} \) in presence of \( 10^{-4} \, \text{M} \) ozone at pH 7

\[ k_{\text{OH}} = 5.0 \times 10^{-11} \, \text{cm}^3 \, \text{molecule}^{-1} \, \text{s}^{-1} \] and \( k_{\text{N}_2\text{O}_5} \approx –5.6 \times 10^{-17} \, \text{cm}^3 \, \text{molecule}^{-1} \, \text{s}^{-1} \) for reaction with \( \text{N}_2\text{O}_5 \) at \( 296 \pm 2 \, \text{K} \) (relative rate method, Atkinson et al. 1990)

\[ \text{photooxidation} \, \frac{\text{t}_{\frac{1}{2}} = 0.802–8.02 \, \text{h}}{\text{based on estimated rate constant for reaction with hydroxyl radical in air}} \] (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 static-flask screening (Tabak et al. 1981)

\[ t_{\frac{1}{2}}(\text{aerobic}) = 5040–45600 \, \text{h}, \text{based on aerobic soil die-away test data at 10–30°C} \] (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991)

\[ k = 0.29 \, \text{h}^{-1} \] in atmosphere (Dragoscu & Friedlander 1989; quoted, Tsai et al. 1991)

\[ k = 0.0027 \, \text{d}^{-1} \] with \( t_{\frac{1}{2}} = 260 \, \text{d} \) for Kidman sandy loam and \( k = 0.0035 \, \text{d}^{-1} \) with \( t_{\frac{1}{2}} = 199 \, \text{d} \) for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990)

\[ t_{\frac{1}{2}}(\text{anaerobic}) = 20160–182400 \, \text{h}, \text{based on estimated unacclimated aqueous aerobic biodegradation half-life} \] (Howard et al. 1991).

Biotransformation: estimated to be \( 1 \times 10^{-10} \, \text{mL} \, \text{cell}^{-1} \, \text{h}^{-1} \) for bacteria (Mabey et al. 1982)

Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants:

\[ k_1 = 1126 \, \text{h}^{-1}; k_2 = 0.343 \, \text{h}^{-1} \] (*Daphnia pulex*, Southworth et al. 1978)

\[ \log k_1 = 3.05 \, \text{h}^{-1}; \log k_2 = -0.46 \, \text{h}^{-1} \] (*Daphnia pulex*, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

\[ k_1 = 113.0 \, \text{h}^{-1}; k_2 = 0.017 \, \text{h}^{-1} \] (*S. heringianus*, Frank et al. 1986)

\[ k_1 = 0.017 \, \text{h}^{-1} \] (*S. heringianus*, Frank et al. 1986)

\[ k_1 = 199.2 \, \text{mL} \, \text{g}^{-1} \, \text{h}^{-1}; k_2 = 0.0012 \, \text{h}^{-1} \] (*4°C, P. h o y i*, Landrum 1988)

\[ k_1 = 3.4–5.3 \, \text{mg} \, \text{g}^{-1} \, \text{h}^{-1}; k_2 = 0.022 \, \text{h}^{-1} \] (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: \( t_{\frac{1}{2}} = 0.68–2.04 \, \text{h} \), 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: \( t_{\frac{1}{2}} = 4.20 \, \text{h} \) under simulated sunlight, \( t_{\frac{1}{2}} = 2.75 \, \text{h} \) under simulated sunlight + ozone (0.2 ppm), \( t_{\frac{1}{2}} = 15.72 \, \text{h} \) under dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);

\[ t_{\frac{1}{2}} = 2.5 \, \text{h} \] with a steady-state concn of tropospheric ozone of \( 2 \times 10^{-9} \, \text{M} \) in clean air (Butković et al. 1983);

\[ \text{photooxidation} \, t_{\frac{1}{2}} = 0.802–8.02 \, \text{h} \] based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: computed near-surface \( t_{\frac{1}{2}} = 0.58 \, \text{h} \) for direct photochemical transformation at latitude 40°N, midday, midsummer. \( t_{\frac{1}{2}} = 4.2 \, \text{h} \) for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning and \( t_{\frac{1}{2}} = 5.9 \, \text{d} \) with sediment-water partitioning (Zepp & Schlotzhauer 1979);

\[ t_{\frac{1}{2}} = 0.68–2.04 \, \text{h} \], based on estimated sunlit photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991);

\[ t_{\frac{1}{2}} = 1.8 \, \text{s} \] in presence of \( 10^{-4} \, \text{M} \) ozone at pH 7 (Butković et al. 1983);

\[ t_{\frac{1}{2}} = 4.2 \, \text{d} \] for summer at 40°N latitude under sunlight (Mill & Mabey 1985);

\[ t_{\frac{1}{2}} = 0.68 \, \text{h} \], based on direct photolysis in sunlight at midday, mid-summer and 40°N latitude (quoted, Zepp 1991);

\[ \text{photolysis} \, t_{\frac{1}{2}} = 3.18 \, \text{h} \] in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: \( t_{\frac{1}{2}} = 10080–91200 \, \text{h} \), based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: reduction \( t_{\frac{1}{2}} = 547 \, \text{h} \) for chemical available pyrene and \( t_{\frac{1}{2}} = 298 \, \text{h} \) for bioavailable pyrene for amphipod, *P. h o y i* in Lake Michigan sediments at 4°C. The uptake clearance from sediment, \( k = (0.019–0.015) \, \text{g} \) of dry sediment–g–1 of organism–h–1, and the rate constants to become biologically unavailable were \( k = 0.0019 \)
h⁻¹ for 10-d aged sediment corresponding to a tᵣᵣ = 365 d and k = 0.0030 h⁻¹ for nonaged sediment corresponding to a tᵣᵣ = 231 h (Landrum 1989).

Soil: tᵣᵣ = 3–35 h (Sims & Overcash 1983; quoted, Bulman et al. 1987);

- tᵣᵣ = 58 d for 5 mg/kg treatment and tᵣᵣ = 48 d for 50 mg/kg treatment (Bulman et al. 1987);
- tᵣᵣ = 5040–45600 h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);
- tᵣᵣ > 50 d (Ryan et al. 1988);
- degradation rate constant, k = 0.0027 d⁻¹ with tᵣᵣ = 260 d for Kidman sandy loam soil and k = 0.0035 d⁻¹ with tᵣᵣ = 199 d for McLaurin sandy loam soil (Park et al. 1990);
- tᵣᵣ = 500 d in soil (Jury et al. 1990);
- tᵣᵣ = 0.4 to more than 90 wk, 8.5 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: depuration tᵣᵣ = 40.8 h in s. heringianus (Frank et al. 1986);

- elimination tᵣᵣ = 4.1–5.5 d from mussel Mytilus edulis; tᵣᵣ = 10.3 d from clam Mya arenaria, tᵣᵣ = 14.4 d from polychaete Abarenicola pacifica, tᵣᵣ = 6.7 d from Oyster, tᵣᵣ = 0.80 d from shrimp, tᵣᵣ = 3.6 d from clam Mercenaria mercenaria (quoted, Meador et al. 1995).

### TABLE 4.1.1.29.1
Reported aqueous solubilities of pyrene at various temperatures

<table>
<thead>
<tr>
<th></th>
<th>Wauchope &amp; Getzen 1972</th>
<th>Schwarz 1977</th>
<th>May et al. 1978a</th>
</tr>
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<td>t/°C</td>
<td>S/g·m⁻³</td>
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<td>0.128</td>
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<td>0.395</td>
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<td>0.534</td>
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<td>0.576</td>
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<td>0.556</td>
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<td>60.7</td>
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<td>ln x</td>
<td>mole fraction</td>
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<td>ΔHₘᵤ(u)/(kJ mol⁻¹) = 15.3</td>
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<td>65.2</td>
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<td>10²·b</td>
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<td>65.2</td>
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<td>c</td>
<td>38.1 ± 0.3</td>
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<tr>
<td>71.9</td>
<td>1.89</td>
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</tr>
<tr>
<td>74.7</td>
<td>2.21</td>
<td></td>
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</tbody>
</table>

Empirical temperature dependence equations:
Wauchope & Getzen (1972): R·ln x = −[Hₘᵤ(u)/(T/K)] + (0.000408)(T/K) – 291.15²−c + b(T/K)
May et al. (1978)– S(µg/kg) = a₁ + b₁·x + c₁·x + d

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TABLE 4.1.1.29.1 (Continued)

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<td>75</td>
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Temp dependence eq. 2
S µg/kg

a −0.0011
b 0.2007
c −1.051
d 50.2

\[ \Delta H_{sol}/(kJ \text{ mol}^{-1}) = 35.44 \]
for temp range 5–30°C

\[ \ln x = A - B/T(K) \]

\[ A = -1.30 \]

\[ B = 5059 \]

temp range 282–305 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

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

1.

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<td>T/K</td>
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<td>∆H_{sub}/(kJ mol⁻¹) = 93.90</td>
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<td>139.97</td>
<td>eq. 1a P/Pa</td>
</tr>
<tr>
<td>130</td>
<td>22.5*</td>
<td>39.34</td>
<td>139.97</td>
<td></td>
</tr>
<tr>
<td>135</td>
<td>29.9*</td>
<td>39.34</td>
<td>139.93</td>
<td></td>
</tr>
<tr>
<td>140</td>
<td>39.5*</td>
<td>39.34</td>
<td>144.90</td>
<td></td>
</tr>
<tr>
<td>145</td>
<td>51.3*</td>
<td>39.45</td>
<td>149.82</td>
<td>68.66</td>
</tr>
<tr>
<td>∆H_{sub}/(kJ mol⁻¹) = 103.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
TABLE 4.1.1.29.2 (Continued)

2.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>inclined-piston gauge</td>
<td>gas saturation-HPLC</td>
<td>electronic manometry</td>
<td>Knudsen effusion</td>
</tr>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
<td><strong>t/°C</strong></td>
<td><strong>P/Pa</strong></td>
</tr>
<tr>
<td>149</td>
<td>63.3*</td>
<td>39.45</td>
<td>3.20 × 10⁻³</td>
</tr>
<tr>
<td>150</td>
<td>66.7*</td>
<td>25.0</td>
<td>6.0 × 10⁻⁴</td>
</tr>
<tr>
<td>152</td>
<td>78.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>155</td>
<td>86.5</td>
<td>eq. 2</td>
<td>P/Pa</td>
</tr>
<tr>
<td>160</td>
<td>110.7</td>
<td>A</td>
<td>12.748</td>
</tr>
<tr>
<td>165</td>
<td>141.6</td>
<td>B</td>
<td>4760.73</td>
</tr>
<tr>
<td>170</td>
<td>178.9</td>
<td>temp range 10–50°C</td>
<td></td>
</tr>
<tr>
<td>175</td>
<td>224.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>280.4</td>
<td>ΔH_{subl}/(kJ mol⁻¹) = 91.20</td>
<td></td>
</tr>
<tr>
<td>185</td>
<td>345.3</td>
<td>B</td>
<td></td>
</tr>
</tbody>
</table>

*supercooled liquid values

reported vapor pressure eq.
see foot note

ΔH_{subl}/(kJ mol⁻¹) = 103.9

temp range: 80.1–139.97°C

ΔH_{subl}/(kJ mol⁻¹) = 97.70

note: ln(P_L/P_S) = 268.6187 – 699.31/(T/K) – 45.6846·ln(T/K) + 0.057217(T/K); in which P_L and P_S are the vapor pressure of supercooled liquid and crystal phase, respectively, at temperature T.

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

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Henry's Law Constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>H/(Pa m^3/mol)</td>
<td>H/(Pa m^3/mol)</td>
</tr>
<tr>
<td>4.1</td>
<td>0.37, 0.49</td>
<td>0.43</td>
</tr>
<tr>
<td>11.0</td>
<td>0.63, 0.76</td>
<td>0.69</td>
</tr>
<tr>
<td>18.0</td>
<td>1.02, 1.19</td>
<td>1.10</td>
</tr>
<tr>
<td>25.0</td>
<td>1.54, 1.89</td>
<td>1.71</td>
</tr>
<tr>
<td>31.0</td>
<td>2.15, 2.80</td>
<td>2.45</td>
</tr>
</tbody>
</table>

\[ \ln K_{AW} = A - B/(T/K) \]

- \[ A = 10.1034 \]
- \[ B = 5160 \]

enthalpy, entropy change:
- \[ \Delta H/(kJ\cdot mol^{-1}) = 42.9 \pm 2.3 \]
- \[ \Delta S/(J\cdot K^{-1}\cdot mol^{-1}) = 84 \]

at 25°C

FIGURE 4.1.1.29.3 Logarithm of Henry’s law constant and K_{OA} 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: C_{16}H_{10}
Molecular Weight: 202.250
Melting Point (°C):
110.19 (Lide 2003)
Boiling Point (°C):
384 (Lide 2003)
Density (g/cm³ at 20°C):
1.252 (0°C, Weast 1982–83, Dean 1985; Lide 2003)
Molar Volume (cm³/mol):
162 (calculated-density, liquid molar volume, Lande & Banerjee 1981)
217.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
18.87 (Ruelle & Kesselring 1997)
18.74 (exptl., Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol 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°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F:
0.146 (mp at 110.19°C)
0.191 (calculated, \( \Delta S_{\text{ fus}} = 49.6 \) J/mol K, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°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 (27°C, shake flask-nephelometry, Davis et al. 1942)
0.265 (shake flask-UV, Klevens 1950)
0.240 (20°C, 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°C, May et al. 1978a,b)
\[ S/(\mu g/kg) = 50.4 + 4.322 \cdot \left( t/°C \right) - 0.1047 \cdot \left( t/°C \right)^2 + 0.0072 \cdot \left( t/°C \right)^3; \] temp range 5–30°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 (15, 25°C, generator column/elution method, average values of 6–7 laboratories, OECD 1981)
0.200 (20°C, quoted, Schmidt-Bleek et al. 1982)
0.190 (20°C, generator column-fluorescence, Hashimoto et al. 1982)
0.203* (24.6°C, generator column-HPLC, measured range 281.25–303.05 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)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

\[
\text{log } (P/Pa) = 5.45017 - 1717.48/(114.025 + t/°C); \text{ temp range } 197–384.2°C (\text{Antoine eq. from reported exptl. data, Boublik et al. 1984})
\]

\[
\text{log } (P/mmHg) = 6.373 - 1756/(114.025 + t/°C); \text{ temp range } 197–384°C (\text{Antoine eq., Dean 1985, 1992})
\]

\[
\text{log } (P/Pa) = 11.96071 - 5348.06/(T/K); \text{ temp range } 298–383 K (\text{Antoine eq.-I, Stephenson & Malanowski 1987})
\]

\[
\text{log } (P/kPa) = 11.35 - 4040/(T/K); \text{ temp range } 503–658 K (\text{Antoine eq.-II, Stephenson & Malanowski 1987})
\]

Henry’s Law Constant (Pa m³/mol 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

\[
\text{log } [H/(Pa m³/mol)] = 8.23 - 2336/(T/K) (\text{Passivirta et al. 1999})
\]

\[
\text{ln } K_{\text{aw}} = -4654.8/(T/K) + 8.42; \Delta H = -79.3 \text{ kJ mol}^{-1} (\text{GC-RT correlation, Lei et al. 2002})
\]
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

1.96 \quad (quoted from Bamford et al. 1999; Dachs & Eisenreich 2000)

0.602 \quad (20°C, selected from reported experimentally measured values, Staudinger & Robers 1996, 2001)

\log K_{AW} = 6.175 – 2868/(T/K) \quad (\text{van't Hoff eq. derived from literature data, Staudinger & Roberts 2001})

### Octanol/Water Partition Coefficient, \( \log K_{OW} \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.22</td>
<td>(RP-TLC-k' correlation, Bruggeman et al. 1982)</td>
</tr>
<tr>
<td>4.47</td>
<td>(HPLC-k' correlation, Harnisch et al. 1983)</td>
</tr>
<tr>
<td>4.84</td>
<td>(RP-HPLC-RT correlation, Chin et al. 1986)</td>
</tr>
<tr>
<td>4.85</td>
<td>(HPLC-RT correlation, Wang et al. 1986)</td>
</tr>
<tr>
<td>5.16</td>
<td>(shake flask/hot stirring-GC, De Bruijn et al. 1989)</td>
</tr>
<tr>
<td>5.20</td>
<td>(recommended, Sangster 1989, 1993)</td>
</tr>
<tr>
<td>5.17</td>
<td>(TLC-RT correlation, De Voogt et al. 1990)</td>
</tr>
<tr>
<td>5.148 \pm 0.077, 5.155 \pm 0.015</td>
<td>(shake flask/hot stirring-GC/HPLC, interlaboratory studies, Brooke et al. 1990)</td>
</tr>
<tr>
<td>5.00</td>
<td>(shake flask-UV spec., Alcorn et al. 1993)</td>
</tr>
<tr>
<td>5.16</td>
<td>(recommended, Hansch et al. 1995)</td>
</tr>
<tr>
<td>5.23 (5.12–5.31)</td>
<td>(shake flask/hot stirring-HPLC/fluorescence, De Maagd et al. 1998)</td>
</tr>
<tr>
<td>5.16</td>
<td>(shake flask-SPME solid-phase micro-extraction; Paschke et al. 1999)</td>
</tr>
<tr>
<td>0.602</td>
<td>(20°C, selected from literature experimentally measured data, Staudinger &amp; Roberts 2001)</td>
</tr>
</tbody>
</table>

\log K_{AW} = 5.485 – 2682/(T/K), \quad (\text{van't Hoff eq. derived from literature data, Staudinger & Roberts 2001})

### Octanol/Air Partition Coefficient, \( \log K_{OA} \) at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.60</td>
<td>(calculated-( K_{OW}/K_{AW} ), Wania &amp; Mackay 1996)</td>
</tr>
<tr>
<td>8.60</td>
<td>(calculated, Finizio et al. 1997)</td>
</tr>
<tr>
<td>8.80*; 8.60</td>
<td>(generator column-GC; calculated-( C_p/C_A ), measured range 0–40°C, Harner &amp; Bidleman 1998)</td>
</tr>
<tr>
<td>\log K_{OA} = –5.94 + 4417/(T/K); temp range 20–40°C</td>
<td>(generator column-GC, Harner &amp; Bidleman 1998)</td>
</tr>
<tr>
<td>8.61</td>
<td>(calculated-S_{oct} and vapor pressure P, Abraham et al. 2001)</td>
</tr>
</tbody>
</table>

### Bioconcentration Factor, \( \log BCF \):

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.18</td>
<td>(calculated as per Kenaga &amp; Goring 1979, Eadie et al. 1982)</td>
</tr>
<tr>
<td>4.90</td>
<td>( P. hovii ), Eadie et al. 1982)</td>
</tr>
<tr>
<td>4.08</td>
<td>(microorganisms-water, calculated from ( K_{OW} ), Mabey et al. 1982)</td>
</tr>
<tr>
<td>3.24</td>
<td>( Daphnia magna ), Newsted &amp; Giesy 1987)</td>
</tr>
<tr>
<td>0.756, 1.079</td>
<td>( Polychaete sp, Capitella capitata ), Bayona et al. 1991)</td>
</tr>
</tbody>
</table>

### Sorption Partition Coefficient, \( \log K_{OC} \) at 25°C or as indicated:

<table>
<thead>
<tr>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.38</td>
<td>(sediments average, Kayal &amp; Connell 1990)</td>
</tr>
<tr>
<td>4.74, 4.62</td>
<td>(RP-HPLC correlation on CIHAC, on PIHAC stationary phases, Szabo et al. 1990b)</td>
</tr>
<tr>
<td>6.30</td>
<td>(Baltic Sea particulate field samples, concn distribution-MS, Broman et al. 1991)</td>
</tr>
<tr>
<td>4.816; 4.81, 4.82</td>
<td>(sediment: concn ratio ( C_{sed}/C_{gw} ); concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter &amp; Alden 1994)</td>
</tr>
<tr>
<td>4.51, 5.05, 4.16</td>
<td>(sediments from Brown’s Lake, Hamlet City Lake, WES reference soil, shake flask-LSC, Brannon et al. 1995)</td>
</tr>
<tr>
<td>6.56, 6.66, 6.08</td>
<td>(marine sediments: Fort Point Channel, Spectacle Island, Peddocks Island, McGroddy &amp; Farrington 1995)</td>
</tr>
<tr>
<td>4.62</td>
<td>(calculated-MCI ( K_{G_a} ), Sabljic et al. 1995)</td>
</tr>
<tr>
<td>5.25 (10°C), 5.22, 5.12 (20°C), 5.05 (35°C), 4.89, 4.96 (45°C)</td>
<td>(log ( K_{DOC} ) - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers &amp; ten Hulscher 1996)</td>
</tr>
<tr>
<td>5.40</td>
<td>(20°C, log ( K_{POC} ) - particulate organic material from lake, Lüers &amp; ten Hulscher 1996)</td>
</tr>
<tr>
<td>4.81, 4.65, 4.80, 4.82; 4.813; 4.727</td>
<td>(4 soils with different organic carbon content ( f_{OC} ), adsorption equilibrium-shake flask-HPLC; calculated-( K_{OW} ); calculated-S, He et al. 1996)</td>
</tr>
<tr>
<td>5.32 (5.29–5.35), 4.89 (4.89–4.90)</td>
<td>(sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask- HPLC/UV, de Maagd et al. 1998)</td>
</tr>
<tr>
<td>4.62, 4.03; 3.40, 4.49, 3.55, 4.53, 4.56</td>
<td>(quoted lit., calculated-( K_{OW} ); HPLC-screening method with different LC-columns, Szabo et al. 1999)</td>
</tr>
</tbody>
</table>
Environmental Fate Rate Constants, k, or Half-Lives, t½:

Vaporization:

Photolysis: direct photochemical transformation t½(calc) = 21 h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis t½ = 160 d and 200 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

t½ = 21 h, atmospheric and aqueous photolysis half life, based on measured sunlight photolysis rate constant in water adjusted for midday summer sunlight at 40°N latitude and t½ = 63 h after adjusting for approximate winter sunlight intensity (Howard et al. 1991);

t½ = 160 d under summer sunlight in surface water (Mill & Mabey 1985);

half-lives on different atmospheric particulate substrates (appr. 25 µg/g on substrate): t½ = 74 h on silica gel, t½ = 23 h on alumina and t½ = 44 h on fly ash (Behymer & Hites 1985);

direct photolysis t½(obs.) = 3.61 h, t½(calc) = 4.78 h, by QSPR in atmospheric aerosol (Chen et al. 2001);

k = (1.76 ± 0.13) × 10⁻¹³ s⁻¹ and t½ = (10.93 ± 0.75)h in diesel particulate matter, photochemical degradation under atmospheric conditions, k = (2.97 ± 0.40) × 10⁻¹³ s⁻¹ and t½ = (6.48 ± 1.03)h in diesel particulate matter/soil mixture, and t½ = 1.6 to 4.15 h in various soil components using a 900-W photo-irradiator as light source; k = (8.69 ± 0.29) × 10⁻¹⁰ s⁻¹ and t½ = (22.16 ± 0.77) h in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation k = 5.0 × 10⁻⁶ 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, kOH for reaction with OH radical, kNO₃ with NO₃ radical and kO₃ with O₃, or as indicated *data at other temperatures and/or the Arrhenius expression see reference:

k(calc) < 3600 M⁻¹ h⁻¹ for singlet oxygen and < 360 M⁻¹ h⁻¹ for peroxy radical (Mabey et al. 1982)

kOH = 5.0 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ and kNO₃ = 1.8 × 10⁻¹⁷ cm³ molecule⁻¹ s⁻¹ for reaction with N₂O₅ at 296 ± 2 K (relative rate method, Atkinson et al. 1990)

photooxidation half-life of 2.02–20.2 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

kOH = 11 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 298 K, measured range 306–366 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 k = 2.2 × 10⁻³ µmol h⁻¹ 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)

t½(aerobic) = 3360–10560 h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; quoted, Howard et al. 1991)

k = 0.19 h⁻¹ in atmosphere (Dragoescu & Friedlander 1989)

k = 0.0018 d⁻¹ with t½ = 377 d for Kidman sandy loam and k = 0.0026 d⁻¹ with t½ = 268 d for McLarin sandy loam all at −0.33 bar soil moisture (Park et al. 1990)

k(an aerobic) = 13440–42240 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

first order k = 0.132 to 0.162 L mg⁻¹ 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 × 10⁻¹⁰ mL cell⁻¹ h⁻¹ (Mabey et al. 1982).

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants:

k₁ = 4.1–6.1 mg g⁻¹ h⁻¹; k₂ = 0.026 h⁻¹ (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

$k_2 = 0.15 \text{ h}^{-1}$ in water with corresponding $t_{1/2} = 4.7 \text{ h}$ and $k_2 = 0.14 \text{ h}^{-1}$ in sediment with corresponding $t_{1/2} = 4.9 \text{ h}$ for copepods $S. knabeni$ in 24-h experiments (Lotufo 1998)

$k_2 = 0.17 \text{ h}^{-1}$ in sediment with corresponding $t_{1/2} = 4.2 \text{ h}$ and $k_2 = 0.09 \text{ h}^{-1}$ in sediment with corresponding $t_{1/2} = 7.4 \text{ h}$ for copepods $Coullana$ sp. in 24-h experiments (Lotufo 1998)

Half-Lives in the Environment:

Air: $t_{1/2} = 2.02–20.2 \text{ h}$, 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 $t_{1/2} = 21 \text{ h}$ for photochemical transformation of a water body (latitude 40°N, midday, midsummer), $t_{1/2} = 160 \text{ d}$ for direct photolysis in a 5-m deep inland water body with no sediment-water partitioning and $t_{1/2} = 200 \text{ d}$ with sediment-water partitioning (Zepp & Schlotzhauer 1979); $t_{1/2} = 21–63 \text{ h}$, based on photolysis half-life in water (Howard et al. 1991); $t_{1/2} = 160 \text{ d}$ for summer sunlight at 40°N latitude (Mill & Mabey 1985).

Groundwater: $t_{1/2} = 6720–21120 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption $t_{1/2} = 8.3 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000). Soil: $t_{1/2} = 44–182 \text{ d}$ (Sims & Overcash 1983; quoted, Bulman et al. 1987); $t_{1/2} = 39 \text{ d}$ for 5 mg/kg treatment and 34 d for 50 mg/kg treatment (Bulman et al. 1987); biodegradation rate constant $k = 0.0018 \text{ d}^{-1}$ with $t_{1/2} = 377 \text{ d}$ for Kidman sandy loam soil, and $k = 0.0026 \text{ d}^{-1}$ with $t_{1/2} = 268 \text{ d}$ for McLaurin sandy loam soil (Park et al. 1990); $t_{1/2} = 3360–10560 \text{ h}$, based on aerobic soil die-away test data at 10–30°C (Howard et al. 1991); $t_{1/2} > 50 \text{ d}$ (Ryan et al. 1988); $t_{1/2} = 17.961 \text{ wk}, 7.8 \text{ yr}$ (Luddington soil, Wild et al. 1991).

Biota: $t_{1/2} = 5 \text{ d}$ depuration half life by oysters (Lee et al. 1978); elimination $t_{1/2} = 6 \text{ d}$ from rainbow trout, $t_{1/2} = 2.0–29.8 \text{ d}$ from mussel $Mytilus edulis$; $t_{1/2} = 8.4 \text{ d}$ from clam $Mya arenaria$, $t_{1/2} = 5.8 \text{ d}$ from polychaete $Aarenicola pacifica$, $t_{1/2} = 5.9 \text{ d}$ from Oyster, $t_{1/2} = 0.8 \text{ d}$ from shrimp (Meador et al. 1995) depuration $t_{1/2} = 4.8 \text{ h}$ in sediment and water for copepod $S. knabeni$, $t_{1/2} = 4.2 \text{ h}$ in sediment and $t_{1/2} = 7.4 \text{ h}$ 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**

\[
S/(\mu g/kg) = a·t^4 + b·t^2 + c·t + d
\]  

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$S/\text{g·m}^{-3}$</td>
</tr>
<tr>
<td>8.1</td>
<td>0.082</td>
</tr>
<tr>
<td>13.2</td>
<td>0.107</td>
</tr>
<tr>
<td>19.7</td>
<td>0.1483</td>
</tr>
<tr>
<td>24.6</td>
<td>0.2027</td>
</tr>
<tr>
<td>29.9</td>
<td>0.2793</td>
</tr>
<tr>
<td>temp dependence eq. 1</td>
<td>b</td>
</tr>
<tr>
<td>given in May et al. 1980</td>
<td>c</td>
</tr>
<tr>
<td>S $\mu g/kg$</td>
<td>d</td>
</tr>
<tr>
<td>a</td>
<td>0.0072</td>
</tr>
<tr>
<td>b</td>
<td>-0.1047</td>
</tr>
<tr>
<td>c</td>
<td>4.322</td>
</tr>
<tr>
<td>d</td>
<td>50.4</td>
</tr>
</tbody>
</table>
**TABLE 4.1.1.30.2**
Reported vapor pressures of fluoranthene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
<th>Equation Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>197.0</td>
<td>653</td>
<td>(1) Data presented in eq. 10.88.</td>
</tr>
<tr>
<td>209.0</td>
<td>1053</td>
<td>(1a) P/mmHg</td>
</tr>
<tr>
<td>228.5</td>
<td>2586</td>
<td>A 12.67</td>
</tr>
<tr>
<td>238.1</td>
<td>3786</td>
<td>B 5357</td>
</tr>
<tr>
<td>247.7</td>
<td>5386</td>
<td>for temp range 25–85°C</td>
</tr>
<tr>
<td>255.0</td>
<td>6586</td>
<td></td>
</tr>
<tr>
<td>261.3</td>
<td>7919</td>
<td>ΔH_{sub}(kJ/mol) = 100</td>
</tr>
<tr>
<td>270.9</td>
<td>10319</td>
<td></td>
</tr>
<tr>
<td>281.5</td>
<td>13386</td>
<td></td>
</tr>
<tr>
<td>305.0</td>
<td>20318</td>
<td></td>
</tr>
<tr>
<td>314.5</td>
<td>27384</td>
<td></td>
</tr>
<tr>
<td>382.9</td>
<td>99058</td>
<td></td>
</tr>
<tr>
<td>384.2</td>
<td>101325</td>
<td></td>
</tr>
</tbody>
</table>

**Tsypkina 1955**

**Hoyer & Peperle 1958**

**Sonnefeld et al. 1983**

**Experimental Data**

- Data presented in eq. 10.88
- P/mmHg
- A 12.67
- B 5357
- for temp range 25–85°C

**Equations**

1. \( \log P = A - \frac{B}{T/K} \)
2. \( \log P = A - \frac{B}{C + t/°C} \)
3. \( \log P = A - \frac{B}{C + T/K} \)
4. \( \log P = A - \frac{B}{T/K} - C \cdot \log (T/K) \)

**Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for fluoranthene.**

**FIGURE 4.1.1.30.1**

**Solubility vs. 1/T**

- Experimental data
- Shaw 1989 (IUPAC recommended)

**∆H_{sub}(kJ/mol) = 100**

- 10.88 2.17 × 10^{-4}
- 10.88 2.05 × 10^{-4}
- 10.88 2.15 × 10^{-4}
- 10.88 2.57 × 10^{-4}
- 20.25 7.07 × 10^{-4}
- 20.25 7.39 × 10^{-4}
- 20.25 7.25 × 10^{-4}
- 20.25 7.63 × 10^{-4}
- 20.25 2.03 × 10^{-3}
- 29.79 1.99 × 10^{-3}
- 29.79 2.17 × 10^{-3}
- 29.80 2.03 × 10^{-3}
- 38.9 5.81 × 10^{-3}
- 38.9 5.67 × 10^{-3}
- 38.9 5.58 × 10^{-3}
- 38.9 5.77 × 10^{-3}
- 38.9 5.46 × 10^{-3}
- 38.9 5.45 × 10^{-3}
- 25.0 1.23 × 10^{-3}

**Temp range 10–50°C**

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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

<table>
<thead>
<tr>
<th>Henry's law constant</th>
<th>log K_{OA}</th>
</tr>
</thead>
<tbody>
<tr>
<td>gas stripping-HPLC/fluo.</td>
<td>gas stripping-GC/MS</td>
</tr>
<tr>
<td>t/°C</td>
<td>H/(Pa m^3/mol)</td>
</tr>
<tr>
<td>10.0</td>
<td>0.26</td>
</tr>
<tr>
<td>20.0</td>
<td>0.64</td>
</tr>
<tr>
<td>35.0</td>
<td>1.63</td>
</tr>
<tr>
<td>40.1</td>
<td>2.38</td>
</tr>
<tr>
<td>45.0</td>
<td>5.84</td>
</tr>
<tr>
<td>55.0</td>
<td>6.23</td>
</tr>
</tbody>
</table>

ln K_{AW} = –ΔH/RT + ΔS/R
R = 8.314 Pa m^3 mol⁻¹ K⁻¹
ΔS/R = 22.16
ΔH/R = 6855.9

ln K_{AW} = A – B/(T/K)
A = 8.4195
B = 4654.8

enthalpy, entropy change:

ΔH/(kJ·mol⁻¹) = 38.7 ± 2.5
ΔS/(J·K⁻¹ mol⁻¹) = 70
TΔS/(kJ·K⁻¹ mol⁻¹) = 54 ± 5

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FIGURE 4.1.1.30.3 Logarithm of Henry's law constant and $K_{OA}$ versus reciprocal temperature for fluoranthene.
4.1.1.31 Benzo[a]fluorene

Common Name: Benzo[a]fluorene
Synonym: 1,2-benzofluorene, 11H-benzo[a]fluorene, chrysofluorene
Chemical Name: benzo[a]fluorene, 1,2-benzofluorene
CAS Registry No: 238-84-6
Molecular Formula: C\textsubscript{17}H\textsubscript{12}
Molecular Weight: 216.227
Melting Point (°C): 189.5 (Lide 2003)
Boiling Point (°C): 405 (Lide 2003)
Density (g/cm\textsuperscript{3} at 20°C):
- 200.9 (Ruelle & Kesselring 1997)
- 239.5 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm\textsuperscript{3}/mol):
- Enthalpy of Fusion, ∆H\textsubscript{fus} (kJ/mol):
  - 3.8, 18.4; 22.2 (126.75, 189.65°C; total phase change enthalpy, Chickos et al. 1999)
- Entropy of Fusion, ∆S\textsubscript{fus} (J/mol 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°C (assuming ∆S\textsubscript{fus} = 56 J/mol K), F: 0.0243 (mp at 189.5°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
- 0.045 (shake flask-fluorescence, Mackay & Shiu 1977)
- 0.045 (average lit. value, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
- 0.00136 (supercooled liquid P\textsubscript{L}, calibrated GC-RT correlation, Lei et al. 2002)
  \[ \log (P\textsubscript{L}/Pa) = -4373/(T/K) + 11.80; \Delta H\textsubscript{vap.} = -83.7 \text{ kJ·mol}^{-1} \] (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol at 25°C or as indicated):
- 2.70* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
\[ \ln K_{AW} = -4113.54/(T/K) + 6.976, \Delta H = 34.2 \text{ kJ mol}^{-1}, \text{measured range 4.1–31°C} \] (gas stripping-GC, Bamford et al. 1999)
Octanol/Water Partition Coefficient, log K\textsubscript{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 K\textsubscript{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K\textsubscript{OC}:
Environmental Fate Rate Constants, k, or Half-Lives, t\textsubscript{1/2}:
Half-Lives in the Environment:
Biota: elimination $t_{1/2} = 10.5$ d from Oyster, $t_{1/2} = 4.2$ d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

### TABLE 4.1.1.31.1
Reported Henry’s law constants of benzo[a]fluorene at various temperatures

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$H/(Pa \ m^3/mol)$</th>
<th>$H/(Pa \ m^3/mol)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>average</td>
<td>0.67, 1.16</td>
<td>0.88</td>
</tr>
<tr>
<td>4.1</td>
<td>1.08, 1.57</td>
<td>1.30</td>
</tr>
<tr>
<td>11.0</td>
<td>1.61., 2.23</td>
<td>1.89</td>
</tr>
<tr>
<td>18.0</td>
<td>2.19, 3.33</td>
<td>2.70</td>
</tr>
<tr>
<td>25.0</td>
<td>2.74, 4.78</td>
<td>3.62</td>
</tr>
</tbody>
</table>

$\ln K_{AW} = A - B/(T/K)$

$A = 6.9762$

$B = 4113.5$

enthalpy, entropy change:

$\Delta H/(kJ \cdot mol^{-1}) = 34.2 \pm 4.9$

$\Delta S/(J \cdot K^{-1} \cdot mol^{-1}) = 58$

at $25°C$

![Henry's law constant vs. 1/T](image)

**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: C_{17}H_{12}
Molecular Weight: 216.227
Melting Point (°C):
212 (Lide 2003)
Boiling Point (°C):
401 (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
200.9 (Ruelle & Kesselring 1997)
239.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
23.4 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{ fus} (J/mol K):
47.78, 50.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.0146 (mp at 212°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.0020 (shake flask-fluorescence, Mackay & Shiu 1977)
0.002 (average lit. value, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°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 × 10^{-6*} (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 71–125°C, Oja & Suuberg 1998)
log (P/Pa) = 36.325 – 14354/(T/K); temp range 344–398 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)
0.00107 (supercooled liquid PL, calibrated GC-RT correlation, Lei et al. 2002)
log (PL/Pa) = –4423/(T/K) + 11.86; ΔH_{ vap.} = –84.7 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ 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 K_{ OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{ oc}:
Environmental Fate Rate Constants, k or Half-Lives, t₁/₂:
Half-Lives in the Environment:
Biota: elimination t₁/₂ = 10.5 d from Oyster, t₁/₂ = 4.3 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

\[
\begin{align*}
\log P &= A - B/(T/K) \\
\ln P &= A - B/(T/K) \\
\log P &= A - B/(C + t/°C) \\
\ln P &= A - B/(C + t/°C) \\
\log P &= A - B/(C + T/K) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K)
\end{align*}
\]

Oja & Suuberg 1998

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>70.92</td>
<td>0.00454</td>
</tr>
<tr>
<td>83.14</td>
<td>0.0188</td>
</tr>
<tr>
<td>97.55</td>
<td>0.0936</td>
</tr>
<tr>
<td>124.4</td>
<td>1.230</td>
</tr>
</tbody>
</table>

mp/K     484–486

eq. 1a    P/Pa
A          36.325
B          14354

for temp range 344–398 K

\[\Delta H_{\text{sub}}/(kJ/mol) = 119.3\]

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: C_{18}H_{12}
Molecular Weight: 228.288
Melting Point (°C):
255.5 (Lide 2003)
Boiling Point (°C):
448 (Weast 1975; Lide 2003)
Density (g/cm³ at 20°C):
1.274 (Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
179.2 (20°C, calculated-density)
250.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} cal/mol:
26.153 (Ruelle & Kesselring 1997)
3.22, 26.15; 29.37 (239.05, 28.25°C, total phase change enthalpy, Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol 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°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.00548 (mp at 255.5°C)
0.00976 (calculated, Passivirta et al. 1999)

Water Solubility (g/m³ or mg/L at 25°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 (27°C, 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°C May et al. 1978a,b)
S/(µg/kg) = 0.609 + 0.0144(t/°C) + 0.0024(t/°C)^2; temp range 5–30°C (generator column-HPLC/UV, May et al. 1978)
0.017 (shake flask-nephelometry, Hollifield 1979)
0.00189* (25.3°C, 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 [S,(mol/L)] = –0.323 – 1369/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°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 × 10−7* (effusion method, extrapolated, De Kruif 1980)
8.4 × 10−7 (effusion method, Hoyer & Peperle 1958; quoted, Mabey et al. 1982)
log (P/mmHg) = 13.07 – 6340/(T/K); temp range 80–145°C (Knudsen effusion method, Hoyer & Peperle 1958)
6.08 × 10−7 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 13.07 – 6340/(T/K); temp range 80–145°C (knudsen effusion method, Hoyer & Peperle 1958
2.29 × 10−4 (supercooled liquid P_L, calculated from Yamasaki et al. 1984, quoted, Finizio et al. 1997)

5.70 × 10−7; 5.84 × 10−5 (quoted solid P_S from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)
log (P_S/Pa) = 12.24 – 5507/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 9.66 – 4139/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P_L/Pa) = 14.848 – 6189/(T/K); temp range 5–50°C (regression eq. from literature data, Shiu & Ma 2000)
log (P_L/Pa) = –50.1566 – 3.4381 × 10^3/(T/K) + 25.178·log(T/K) – 2.462 × 10−2·(T/K) + 7.1044 × 10−6·(T/K^2); temp range 531–979 K (vapor pressure eq., Yaws 1994)
1.70 × 10−4 (supercooled liquid P_L, calculated from Yamasaki et al. 1984, quoted, Finizio et al. 1997)

Henry’s Law Constant (Pa m^3/mol at 25°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 & Pawlisyn 1993)
0.53* (gas stripping-GC, measured range 4.1–31°C, Bamford et al. 1999)
ln K_{AW} = –12136.2/(T/K) + 32.235, \Delta H = 100.9 kJ mol−1, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
log (H/(Pa m^3/mol)) = 9.98 – 2770/(T/K) (Passivirta et al. 1999)
0.53 (quoted, Dachs & Eisenreich 2000)

Octanol/Water Partition Coefficient, log K_{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 ± 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/fluor., De Maagd et al. 1998)
5.78 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)
10.40 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.44 (calculated, Finizio et al. 1997)

Octanol/Air Partition Coefficient, log K_{OA}:
4.31 (P. hoya, Eadie et al. 1982)
4.72 (microorganisms-water, calculated from K_{OW}, Mabey et al. 1982)
3.785 (Daphnia magna, Newsted & Giesy 1987)
1.17, 0.792 (Polychaete sp, Capitella capitata, Bayona et al. 1991)

Bioconcentration Factor, log BCF:
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 K_{OC}, Broman et al. 1991)
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5.79 (5.74–5.83), 5.40 (5.35–5.50) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/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°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, $t_{1/2}$:

Volatilization:
Photolysis: calculated $t_{1/2} = 4.4$ h of direct sunlight photolysis for 50% conversion at 40°N latitude of midday in midsummer: 4.4 h in near-surface water; (Herbes et al. 1980)
direct photochemical transformation $t_{1/2}^{(calc)} = 4.4$ h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 13$ d and 68 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

$t_{1/2} = 13$ d in 5-m deep inland water and $t_{1/2} = 68$ d in inland water with sediment partitioning (Zepp & Schlotzhauer 1979)
half-lives on different atmospheric particulate substrates (appr. 25 µg/g on substrate): $t_{1/2} = 100$ h on silica gel, $t_{1/2} = 78$ h on alumina and $t_{1/2} = 38$ h on fly ash (Behymer & Hites 1985)
first order daytime decay constants:: $k = 0.0056$ min$^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0090$ min$^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988)
photodegradation $k = 7.07 \times 10^{-1}$ min with $t_{1/2} = 1.63$ h in ethanol-water (1:1, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)

$k^{(exp)} = 0.00707$ min$^{-1}$ with the calculated $t_{1/2} = 1.63$ h and the predicted $k = 0.0114$ min$^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

$k = 1.01–1.30$ min$^{-1}$ in natural water system by UV and sunlight (Yu et al. 1999)

$t_{1/2}^{(obs)} = 1.58$ h, $t_{1/2}^{(calc)} = 1.34$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
photochemical degradation $k = (1.60 \pm 0.08) \times 10^{-5}$ s$^{-1}$ and $t_{1/2} = (11.99 \pm 0.53)$h in diesel particulate matter under atmospheric conditions; $k = (2.29 \pm 0.22) \times 10^{-5}$ s$^{-1}$ and $t_{1/2} = (8.41 \pm 0.91)$h in diesel particulate matter/soil mixture, and $t_{1/2} = 1.69–8.82$ h in various soil components using a 900-W photo-irradiator as light source; $k = (4.76 \pm 0.40) \times 10^{-5}$ s$^{-1}$ and $t_{1/2} = (405.26 \pm 37.27)$h in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001)

Photodegradation $k = 9.0 \times 10^{-5}$ s$^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: $t_{1/2} = 2.6$ h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

$k > 1 \times 10^{6}$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 1 \times 10^{8}$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982); photooxidation $t_{1/2} = 0.802–0.802$ 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 $t_{1/2} = 8904–24000$ h, based on aerobic soil dieaway test data (Howard et al. 1991)
rate constants $k = 0.0019$ d$^{-1}$ with $t_{1/2} = 371$ d for Kidman sandy loam and $k = 0.0018$ d$^{-1}$ with $t_{1/2} = 387$ d for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990)
anaerobic $t_{1/2} = 35616–96000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: estimated to be $1 \times 10^{-10}$ mL cell$^{-1}$ h$^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 0.35–0.71$ mg g$^{-1}$ h$^{-1}$; $k_2 = 0.15$ h$^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:
Air: $t_{1/2} = 0.802–0.802$ h, based on estimated photooxidation half-life in air (Howard et al. 1987);
t_{1/2} = 1.3 h for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated rate constant k = 0.0092 min\(^{-1}\) at 1 cal cm\(^{-2}\) min\(^{-1}\), 10 g/m\(^3\) H\(_2\)O and 20°C (Kamens et al. 1988).

Surface water: photolysis t_{1/2} = 4.4 h near surface water, t_{1/2} = 13 d and 68 d in 5-m deep water body without and with sediment-water partitioning in full summer day, 40°N; photosensitized oxygenation t_{1/2} = 2.6 h at near surface water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

t_{1/2} \approx 4.4–13 h, based on photolysis half-life in water (Howard et al. 1991);
photolysis t_{1/2} = 1.63 h in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996);
photolysis t_{1/2} = 533–693 min at 18°C in natural water system by UV and sunlight illumination (Yu et al. 1999).

Groundwater: t_{1/2} = 17808–48000 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption t_{1/2} = 31.9 d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: t_{1/2} > 5.5 d (Sims & Overcash 1983; quoted, Bulman et al. 1987);

t_{1/2} = 328 d for 5 mg/kg treatment and t_{1/2} = 224 d for 50 mg/kg treatment (Bulman et al. 1987);
biodegradation rate constant l = 0.0019 d\(^{-1}\) with t_{1/2} = 371 d for Kidman sandy loam soil, and k = 0.0018 h\(^{-1}\) with t_{1/2} = 387 d for McLaurin sandy loam soil (Park et al. 1990);

t_{1/2} = 8904–24000 h, based on aerobic soil die-away test data (Howard et al. 1991);

t_{1/2} > 50 d (Ryan et al. 1988).

Biota: elimination t_{1/2} = 5.0–14.2 d from mussel Mytilus edulis; t_{1/2} = 15.1 d from Oyster, t_{1/2} = 4.3 d from clam Mercenaria mercenaria, t_{1/2} = 3.3 d from clam Macoma balthica (quoted, Meador et al. 1995).

**TABLE 4.1.133.1**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (µg/kg)</th>
<th>Temperature (°C)</th>
<th>Solubility (µg/kg)</th>
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<tr>
<td>25</td>
<td>0.0018</td>
<td>5.0</td>
<td>0.0071</td>
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<tr>
<td>29</td>
<td>0.0022</td>
<td>11.0</td>
<td>0.00080</td>
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<tr>
<td>temp dependence eq. 1</td>
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<tr>
<td>S</td>
<td>µg/kg</td>
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<td>0.00168</td>
</tr>
<tr>
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<td>25.3</td>
<td>0.00189</td>
</tr>
<tr>
<td>b</td>
<td>0.0024</td>
<td>temp dependence eq. 1 given in May 1980</td>
<td></td>
</tr>
<tr>
<td>c</td>
<td>-0.0144</td>
<td>a</td>
<td>0</td>
</tr>
<tr>
<td>d</td>
<td>0.69</td>
<td>b</td>
<td>0.0024</td>
</tr>
<tr>
<td></td>
<td></td>
<td>c</td>
<td>-0.0144</td>
</tr>
<tr>
<td></td>
<td></td>
<td>d</td>
<td>0.69</td>
</tr>
<tr>
<td>ΔΗ(_{sol})(kJ mol(^{-1})) = 41.25</td>
<td></td>
<td>ΔΗ(_{sol})(kJ mol(^{-1})) = 41.25</td>
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</tr>
<tr>
<td>measured between 5–30°C</td>
<td></td>
<td>measured between 5–30°C</td>
<td></td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Vapor pressure</th>
<th>Henry’s law constant</th>
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<tr>
<td></td>
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</tr>
<tr>
<td></td>
<td>Hoyer &amp; Peperle 1958</td>
</tr>
<tr>
<td>t/°C</td>
<td>$P/\text{Pa}$</td>
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<tr>
<td>data presented by equation</td>
<td>117.31</td>
</tr>
<tr>
<td>log $P/\text{mmHg} = A - B/(T/\text{K})$</td>
<td>124.84</td>
</tr>
<tr>
<td>A</td>
<td>13.07</td>
</tr>
<tr>
<td>B</td>
<td>6340</td>
</tr>
<tr>
<td>temp range 80–145°C</td>
<td>135.26</td>
</tr>
<tr>
<td></td>
<td>137.39</td>
</tr>
<tr>
<td>$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.8$</td>
<td>139.22</td>
</tr>
<tr>
<td></td>
<td>140.81</td>
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<tr>
<td></td>
<td>142.23</td>
</tr>
<tr>
<td></td>
<td>143.51</td>
</tr>
<tr>
<td>$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.5$</td>
<td>25.0</td>
</tr>
<tr>
<td></td>
<td>$\Delta S/(\text{J}/\text{K}/\text{mol}) = 268$ at 25°C</td>
</tr>
</tbody>
</table>

|                | de Kruif 1980          |
| t/°C           | $P/\text{Pa}$         |
|                | 117.31 | 0.1 |
|                | 124.84 | 0.2 |
| A              | 13.07 | 129.38 |
| B              | 6340 | 0.3 |
| temp range 80–145°C | 135.26 | 0.5 |
|                | 137.39 | 0.6 |
| $\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.8$ | 25.0 | $5.7 \times 10^{-7}$ |
|                | $\Delta S/(\text{J}/\text{K}/\text{mol}) = 268$ at 25°C |

|                | Bamford et al. 1999    |
| t/°C           | $H/(\text{Pa m}^3/\text{mol})$ | $H/(\text{Pa m}^3/\text{mol})$ |
|                | average                |
| $\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.5$ | 114.84 | 0.1 |
|                | 117.31 | 0.1 |
|                | 124.84 | 0.2 |
| A              | 13.07 | 129.38 |
| B              | 6340 | 0.3 |
| temp range 80–145°C | 135.26 | 0.5 |
|                | 137.39 | 0.6 |
| $\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.8$ | 25.0 | $5.7 \times 10^{-7}$ |
|                | $\Delta S/(\text{J}/\text{K}/\text{mol}) = 268$ at 25°C |

$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 118.8$

$\Delta S/(\text{J}/\text{K}/\text{mol}) = 268$

at 25°C
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:** C\textsubscript{18}H\textsubscript{12}  
**Molecular Weight:** 228.288  
**Melting Point (°C):**  
\[197.8\] (Lide 2003)  
**Boiling Point (°C):**  
\[425\] (Weast 1982–83; Dean 1985; Pearlman et al. 1984; Budavari 1989; Lide 2003)  
**Density (g/cm\textsuperscript{3} at 20°C):**  
\[1.302\] (Dean 1985; Budavari 1989)  
**Molar Volume (cm\textsuperscript{3}/mol):**  
\[211.8\] (Ruelle & Kesselring 1997)  
\[250.8\] (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, \(\Delta H_{\text{fus}}\) (kJ/mol):**  
\[24.74\] (exptl., Chickos et al. 1999)  
**Entropy of Fusion, \(\Delta S_{\text{fus}}\) (J/mol K):**  
\[52.53, 44.1\] (exptl., calculated-group additivity method, Chickos et al. 1999)  
**Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{fus}} = 56\) J/mol K), F:**  \[0.0202\] (mp at 197.8°C)  
**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *) are compiled at the end of this section):**  
\[0.0388\] (27°C, nephelometry, Davis et al. 1942)  
\[0.043\] (shake flask-UV, Kleevens 1950)  
\[0.043\] (shake flask-fluorescence, Mackay & Shiu 1977)  
\[0.0049^*\] (20.5°C, 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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *) are compiled at the end of this section):**  
\[\log (P/\text{mmHg}) = 12.89 - 6154/(T/K);\text{ temp range: } 65-125°C\] (Knudsen effusion method, Hoyer & Peperle 1958)  
\[2.30 \times 10^{-6}\textsuperscript{*} (effusion, De Kruif 1980)\]  
\[3.85 \times 10^{-3}\textsuperscript{*} \text{ (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)}\]  
\[\log (P_{L}/\text{kPa}) = 9.435 - 5620/(T/K);\text{ temp range: } 363-468 K\] (Antoine eq.-I, Stephenson & Malanowski 1987)  
\[1.17 \times 10^{-2}\textsuperscript{*} \text{ (extrapolated-Antoine eq.-II, supercooled liquid \(P_{L}\), Stephenson & Malanowski 1987)}\]  
\[\log (P_{L}/\text{kPa}) = 6.8974 - 3527/(T/K);\text{ temp range: } 600-720 K\] (Antoine eq.-II, Stephenson & Malanowski 1987)  
\[2.39 \times 10^{-4}\textsuperscript{*} \text{ (supercooled liquid \(P_{L}\), GC-RT correlation, Lei et al. 2002)}\]  
\[\log (P_{L}/\text{Pa}) = -4624/(T/K) + 11.89;\text{ \(\Delta H_{\text{vap.}} = -88.5\) kJ·mol}^{-1}\text{ (GC-RT correlation, Lei et al. 2002)}\]  
**Henry’s Law Constant (Pa m\textsuperscript{3}/mol):**  
\[5.45\] (shake flask-UV, Karickhoff et al. 1979)  
\[5.49\] (HPLC-RT correlation, Wang et al. 1986)  
\[5.84\] (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 $K_{ow} = 1.313 + 1138.55/(T/K)$; temp range 5–55°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 $K_{OA}$:

Bioconcentration Factor, log BCF:

3.96 (Daphnia magna, Newsted & Giesy 1987)

Sorption Partition Coefficient, log $K_{OC}$:

6.90 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
4.0 (predicted dissolved log $K_{OC}$, 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°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, $t_\frac{1}{2}$:

Half-Lives in the Environment:

Biota: elimination $t_\frac{1}{2} = 2$ d from rainbow trout, $t_\frac{1}{2} = 4.4$ d from clam Mya arenaria, $t_\frac{1}{2} = 8.0$ d from mussel Mytilus edulis, $t_\frac{1}{2} = 14.4$ d from polychaete Abarenicola pacifica, $t_\frac{1}{2} = 21.7$ d from Oyster, $t_\frac{1}{2} = 2.4$ 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

$$S/(\mu g/kg) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d$$

| Aqueous solubility | Vapor pressure |
|--------------------|---------------|-----------------|-----------------|
| generator column-HPLC | effusion | torsion, weighing effusion |
| $t/^\circ C$ | $S/\mu g.m^{-3}$ | $t/^\circ C$ | $P/Pa$ | $t/^\circ C$ | $P/Pa$ |
| 8.0 | 0.00299 | data presented by | | | |
| 12.0 | 0.00393 | log P/mmHg = A – B/(T/K) | | | |
| 14.8 | 0.00339 | A | 12.89 | | |
| 20.5 | 0.00489 | B | 6154 | | |
| 27.3 | 0.00765 | temp range 65–125°C | | | |
| 28.2 | 0.00811 | $\Delta H_{subl}/(kJ \cdot mol^{-1}) = 114.6$ | | | |

Temp dependence eq. 1 given in May 1980

S $\mu g/kg$

| | | | | |
| a | -0.0002 | | 25.0 | 2.3 $\times 10^{-4}$ |
| b | 0.0250 | | | extrapolated |
| c | -0.4250 | | | |
| d | 4.89 | | $\Delta H_{subl}/(kJ \cdot mol^{-1}) = 115.2$ |

$\Delta H_{subl}/(kJ \cdot mol^{-1}) = 41.25$

measured between 5–30°C
FIGURE 4.1.34.1 Logarithm of mole fraction solubility and vapor pressure versus reciprocal temperature for triphenylene.
4.1.1.35  *o*-Terphenyl

![Chemical Structure](image)

Common Name: *o*-Terphenyl
Synonym: 1,2-diphenyl benzene
Chemical Name:
CAS Registry No: 84-15-1
Molecular Formula: C\(_{18}\)H\(_{14}\), 1,2-(C\(_6\)H\(_5\))\(_2\)C\(_6\)H\(_4\)
Molecular Weight: 230.304
Melting Point (°C): 56.2 (Lide 2003)
Boiling Point (°C): 332 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm\(^3\)):

Molar Volume (cm\(^3\)/mol):
225.4 (93°C, Stephenson & Malanowski 1987)
273.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):
17.2 (Chickos et al. 1999)

Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):
52.3, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)

Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56\) J/mol K), \(F\): 0.494 (mp at 56.2°C)

Water Solubility (g/m\(^3\) or mg/L at 25°C):
1.24 (vapor saturation-spectrophotometry, Akiyoshi et al. 1987)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\[
\log (P/kPa) = 6.29308 - [2160.24/(-106.38 + (T/K))]; \text{ temp range 462–650 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)}
\]
\[
\log (P/mmHg) = -8.0641 - 4.0928 \times 10^3/(T/K) + 9.1076 \log (T/K) - 1.6326 \times 10^{-2} \cdot (T/K) + 6.0467 \times 10^{-6} \cdot (T/K)^2; \text{ temp range 329–891 K (vapor pressure eq., Yaws 1994)}
\]

Henry’s Law Constant (Pa·m\(^3\)/mol):

Octanol/Water Partition Coefficient, log \(K_{\text{ow}}\):

Octanol/Air Partition Coefficient, log \(K_{\text{oa}}\):

Bioconcentration Factor, log BCF or log \(K_b\):

Sorption Partition Coefficient, log \(K_{\text{oc}}\):

Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{\frac{1}{2}}\):

Half-Lives in the Environment:
Air:
Surface water: a first order reduction process in river water with an estimated \(t_{\frac{1}{2}} = 0.6\) d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).

Ground water:

Sediment:

Soil:

Biota:
4.1.1.36  \textit{m}-Terphenyl

![Chemical Structure](image)

Common Name: \textit{m}-Terphenyl
Synonym: 1,3-diphenyl benzene
Chemical Name:
CAS Registry No: 92-06-8
Molecular Formula: C_{18}H_{14}, 1,3-(C_{6}H_{5})_{2}C_{6}H_{4}
Molecular Weight: 230.304
Melting Point (°C): 87 (Lide 2003)
Boiling Point (°C): 363 (Lide 2003)
Density (g/cm³ at 20°C): 1.199 (Lide 2003)
Molar Volume (cm³/mol):
227 (93°C, Stephenson & Malanowski 1987)
192.1 (20°C, calculated-density)
273.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
22.59 (Chickos et al. 1999)
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
62.76, 73.9 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), F: 0.246 (mp at 87°C)
Water Solubility (g/m³ or mg/L at 25°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* (24.99°C, generator column-HPLC/fluorescence, Reza et al. 2002)
\(\ln x = (-2.62 \pm 0.91) + (-5134 \pm 271)/(T/K)\); temp range 278–323.13 K (Reza et al. 2002)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
\(\log (P/kPa) = 6.48808 - [2445.98/(–102.76 + (T/K))];\) temp range 462–691 K (Antoine eq., liquid phase, Stephenson & Malanowski 1987)
\(\log (P/mmHg) = -14.7175 - 4.3577 \times 10^3/(T/K) + 11.935 \log (T/K) - 1.8441 \times 10^{-2}\times(T/K) + 6.437 \times 10^{-6}\times(T/K)^2;\) temp range 360–925 K (vapor pressure eq., Yaws 1994)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, \(\log K_{ow}\):
Octanol/Air Partition Coefficient, \(\log K_{oa}\):
Bioconcentration Factor, \(\log BCF\) or \(\log K_{b}\):
Sorption Partition Coefficient, \(\log K_{sc}\):
Environmental Fate Rate Constants, k and Half-Lives, \(t_{1/2}\):
Half-Lives in the Environment:
Air:
Surface water: a first order reduction process in river water with an estimated \(t_{1/2} = 0.6\) d for terphenyl in Rhine River, isomer unspecified (Zoeteman et al. 1980).
Ground water:
Sediment:
Soil:
Biota:

<table>
<thead>
<tr>
<th>TABLE 4.1.1.36.1</th>
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<tr>
<td>Reported aqueous solubilities of m-terphenyl at various temperatures</td>
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<tr>
<td>Reza et al. 2002</td>
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<td>generator column-HPLC</td>
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<td>( t/°C )</td>
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<td>30.0</td>
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<td>35.0</td>
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</tbody>
</table>

**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

\[ \begin{array}{c}
\text{Common Name:} \quad p \text{-Terphenyl} \\
\text{Synonym:} \quad 1,4\text{-diphenyl benzene} \\
\text{Chemical Name:} \quad p\text{-terphenyl} \\
\text{CAS Registry No:} \quad 92-94-4 \\
\text{Molecular Formula:} \quad \text{C}_{18}\text{H}_{14} \quad \text{1,4-}\left(\text{C}_{6}\text{H}_{5}\right)_{2}\text{C}_{6}\text{H}_{4} \\
\text{Molecular Weight:} \quad 230.304 \\
\text{Melting Point} (\text{°C}): \\
\quad 213.9 \quad \text{(Lide 2003)} \\
\text{Boiling Point} (\text{°C}): \\
\quad 376 \quad \text{(Lide 2003)} \\
\text{Density} (\text{g/cm}^3): \\
\text{Molar Volume} (\text{cm}^3/\text{mol}): \\
\quad 262.0 \quad \text{(315.6°C, Stephenson & Malanowski 1987)} \\
\quad 273.2 \quad \text{(calculated-Le Bas method at normal boiling point)} \\
\text{Enthalpy of Fusion, } \Delta H_{\text{fus}} (\text{kJ/mol}): \\
\quad 0.3, 35.3; 35.6 \quad \text{(~-79.55, 213.85°C; total phase change enthalpy, Chickos et al. 1999)} \\
\text{Entropy of Fusion, } \Delta S_{\text{fus}} (\text{J/mol K}): \\
\quad 74.1, 73.9 \quad \text{(~exptl., calculated-group additivity method, total phase change entropy, Chickos et al. 1999)} \\
\text{Fugacity Ratio at 25°C (assuming } \Delta S_{\text{fus}} = 56 \text{ J/mol K, F: 0.014 (mp at 213.9°C)} \\
\text{Water Solubility} (\text{g/m}^3 \text{ or mg/L at 25°C}): \\
\quad 1.80 \quad \text{(vapor saturation-spectrophotometry, Akiyoshi et al. 1987)} \\
\text{Vapor Pressure (Pa at 25°C and reported temperature dependence equations):} \\
\quad 4.86 \times 10^{-6} \quad \text{(extrapolated from solid, Stephenson & Malanowski 1987)} \\
\text{log (P}_v/\text{kPa}) = 12.515 – 6210/(T/K); \text{ temp range 338–431 K (Antoine eq.-I, solid phase, Stephenson & Malanowski 1987)} \\
\quad 1.78 \times 10^{-5} \quad \text{(P}_l \text{ extrapolated from liquid state, Stephenson & Malanowski 1987)} \\
\text{log (P}_l/\text{kPa}) = 6.16107 – [2125.84/(-145.29 + (T/K)); \text{ temp range 499–700 K (Antoine eq.-II, liquid phase, Stephenson & Malanowski 1987)} \\
\text{log (P}/\text{mmHg) = –39.6342 – 3.2661 \times 10^4/(T/K) + 21.08\log \text{(T/K)} – 2.2574 \times 10^2/(T/K) + 6.902 \times 10^4/(T/K)^2; \text{ temp range 485–926 K (vapor pressure eq., Yaws 1994)} \\
\text{5.40 \times 10^{-4}} \quad \text{(supercooled liquid P}_l \text{, GC-RT correlation, Lei et al. 2002)} \\
\text{log (P}_l/\text{Pa}) = –4135/(T/K) + 10.60; \Delta H_{\text{vap.}} = –79.2 \text{ kJ/mol}^{-1} \quad \text{(GC-RT correlation, Lei et al. 2002)} \\
\text{Henry’s Law Constant (Pa·m}^3/\text{mol):} \\
\text{Octanol/Water Partition Coefficient, log K}_{\text{ow}}: \\
\quad 6.03, 5.88 \quad \text{(HPLC-RV correlation, Garst 1984)} \\
\quad 6.03 \pm 0.50 \quad \text{(recommended, Sangster 1989)} \\
\text{Octanol/Air Partition Coefficient, log K}_{\text{oa}}: \\
\text{Bioconcentration Factor, log BCF or log K}_{\text{b}}: \\
\text{Sorption Partition Coefficient, log K}_{\text{OC}}: \\
\text{Environmental Fate Rate Constants, k and Half-Lives, } t_{\frac{1}{2}}: \\
\text{© 2006 by Taylor & Francis Group, LLC}
Half-Lives in the Environment:

Air:
Surface water: a first order reduction process in river water with an estimated $t_{1/2} = 0.6$ 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: \(\text{C}_{18}\text{H}_{12}\)
Molecular Weight: 228.288
Melting Point (°C):
357 (Lide 2003)
Boiling Point (°C):
450 (sublimation, Bjørseth 1983; Lide 2003)
Density (g/cm\(^3\) at 20°C):
Molar Volume (cm\(^3\)/mol):
211.8 (Ruelle & Kesselring 1997)
250.8 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):
38.64 (Ruelle & Kesselring 1997)
Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K): Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56 \text{ J/mol K}\), F: 0.000553 (mp at 357°C)
Water Solubility (g/m\(^3\) or mg/L at 25°C or as indicated):
0.0010 (27°C, 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 & Shiui 1977)
0.044 (shake flask-nephelometry, Hollifield 1979)
0.00103 (lit. mean, Pearlman et al. 1984)
Vapor Pressure (Pa at 25°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 \text{(effusion method, De Kruif 1980)}
3.70 \times 10^{-8} \quad \text{(extrapolated-Antoine eq., Stephenson & Malanowski 1987)}
\log (P/Pa) = 11.505 – 6540/(T/K); temp range 376–489 K (Antoine eq., Stephenson & Malanowski 1987)
2.31 \times 10^{-8}^* \quad \text{(gas saturation, extrapolated-Antoine eq. derived from explt. data, temp range 113–199°C, Oja & Suuberg 1998)}
\log (P/Pa) = 33.594 – 15151/(T/K); temp range 368–472 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)
Henry’s Law Constant (Pa m\(^3\)/mol):
Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):
5.90 \quad \text{(shake flask-UV, concn. ratio, Karickhoff et al., 1979)}
6.02 \quad \text{(HPLC-k’ correlation, McDuffie 1981)}
5.76 \quad \text{(HPLC-RT correlation, Wang et al. 1986)}
5.76 \quad \text{(recommended, Sangster 1989, 1993)}
5.84 \quad \text{(TLC retention time correlation, De Voogt et al. 1990)}
5.90 \quad \text{(shake flask-HPLC, De Voogt et al. 1990)}
5.90 \quad \text{(recommended, Hansch et al 1995)}
Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\):
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log $K_{OC}$:
5.81 (sediment, batch equilibrium-sorption isotherms by GC/UV, Karickhoff et al. 1979)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatile:

Photolysis: direct photochemical transformation $t_{1/2} = 0.034$ h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 0.20$ d and 0.95 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

Photodegradation $k = 0.051$ min$^{-1}$ and $t_{1/2} = 0.23$ h in ethanol-water (1:1, v/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 $k$ (exptl) = 0.051 min$^{-1}$ with the calculated $k$ = 0.051 min$^{-1}$ and $t_{1/2} = 0.23$ h and the predicted $k$ (calc) = 0.0355 min$^{-1}$ calculated by QSPR in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)

Direct photolysis $t_{1/2} = 0.92$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001).

Oxidation: $t_{1/2} = 2.6$ h for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: direct photolysis $t_{1/2} = 0.92$ h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Surface water: photolysis $t_{1/2} = 0.034$ h near surface water, $t_{1/2} = 0.20$ d and 0.95 d in 5-m deep water body without and with sediment-water partitioning in full summer day, 40°N; photosensitized oxygenation $t_{1/2} = 2.6$ h at near surface water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979).

Photolysis $t_{1/2} = 0.23$ h in aqueous solution when irradiated with a 500W 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

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
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<tr>
<td>147.35</td>
<td>0.1</td>
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<tr>
<td>155.46</td>
<td>0.2</td>
</tr>
<tr>
<td>160.35</td>
<td>0.3</td>
</tr>
<tr>
<td>163.89</td>
<td>0.4</td>
</tr>
<tr>
<td>166.67</td>
<td>0.5</td>
</tr>
<tr>
<td>168.97</td>
<td>0.6</td>
</tr>
<tr>
<td>170.94</td>
<td>0.7</td>
</tr>
<tr>
<td>172.65</td>
<td>0.8</td>
</tr>
<tr>
<td>173.98</td>
<td>0.9</td>
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<tr>
<td>175.65</td>
<td>1.0</td>
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</table>

<table>
<thead>
<tr>
<th>de Kruif 1980</th>
<th>Oja &amp; Suuberg 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
</tr>
<tr>
<td>113.4</td>
<td>0.00344</td>
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<td>128.78</td>
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<td>139.56</td>
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<tr>
<td>145.44</td>
<td>0.0496</td>
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<tr>
<td>160.69</td>
<td>0.322</td>
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<tr>
<td>172.88</td>
<td>0.584</td>
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<tr>
<td>198.99</td>
<td>4.81</td>
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<tr>
<td>mp/K</td>
<td>630</td>
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TABLE 4.1.1.38.1 (Continued)

<table>
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<tr>
<th></th>
<th>de Kruif 1980</th>
<th>Oja &amp; Suuberg 1998</th>
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<tr>
<td></td>
<td>torsion-, weighing effusion</td>
<td>Knudsen effusion</td>
</tr>
<tr>
<td>t/°C</td>
<td>P/Pa</td>
<td>t/°C</td>
</tr>
<tr>
<td>25.0</td>
<td>$9.7 \times 10^{-9}$ eq. 1a</td>
<td>35.594 eq. 1a</td>
</tr>
<tr>
<td>$\Delta H_{\text{sub}}/(kJ \text{ mol}^{-1})$ = 155.0</td>
<td>extrapolated</td>
<td>A</td>
</tr>
</tbody>
</table>

for temp range 386–472 K

$\Delta H_{\text{sub}}/(kJ \text{ mol}^{-1})$ = 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, tetrathene
Chemical Name: 1,2-benzanthracene
CAS Registry No: 56-55-3
Molecular Formula: C_{18}H_{12}
Molecular Weight: 228.288
Melting Point (°C):
160.5  (Lide 2003)
Boiling Point (°C):
438  (Lide 2003)
Density (g/cm³ at 20°C):
1.2544  (Mailhot & Peters 1988)
Molar Volume (cm³/mol):
211.8  (Ruelle & Kesselring 1997; Passivirta et al. 1999)
248.3  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
21.38  (Ruelle & Kesselring 1997; Chickos et al. 1999)
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
49.23, 44.1  (exptl., calculated-group additivity method, Chickos et al. 1999)
49.2  (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
0.0468  (mp at 160.5°C)
0.040  (calculated, assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K, Mackay et al. 1980)
0.0661  (calculated, \( \Delta S_{\text{fus}} = 49.2 \) J/mol K, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.011  (27°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)
\( S/(\mu g/kg) = 1.74 + 0.1897 \cdot (t/°C) + 0.0031 \cdot (t/°C)^2 + 0.0003 \cdot (t/°C)^3, \) temp range 5–30°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°C, May 1980)
0.0086*  (generator column-HPLC, measured range 6.9–29.7°C, May et al. 1983)
0.00935*  (generator column-fluo., measured range 10–30°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°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)
\[ \log [S_l/(mol/L)] = -0.326 - 1119/(T/K) \] (supercooled liquid, Passivirta et al. 1999)
\[ \ln x = -3.060466 - 5354.51/(T/K) \] (regression eq. of literature data, Shiu & Ma 2000)
Vapor Pressure (Pa at 25°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}  (20°C, Hoyer & Peperle 1958)
\[ \log (P/mmHg) = 13.68 - 6250/(T/K); \] temp range 60–120°C (Knudsen effusion method, Hoyer & Peperle 1958)
2.17 × 10⁻⁵ (solid, extrapolated from Antoine eq., Kelley & Rice 1964; quoted, Bidleman 1984)
log (P/mmHg) = 11.528 – 5461/(T/K); temp range: 104–127°C (effusion method, Kelley & Rice 1964)
3.87 × 10⁻⁷ (effusion method, Wakayama & Inokuchi 1967)
1.47 × 10⁻⁵ (solid, effusion method, extrapolated-Antoine eq., Murray et al. 1974)
log (P/mmHg) = 10.045 – 5929/(T/K); temp range: 330–390 K (effusion method, Murray et al. 1974)
6.67 × 10⁻⁷ (20°C, effusion, Pupp et al. 1974)
7.30 × 10⁻⁶ (effusion method, De Kruijf 1980)
6.67 × 10⁻⁷ (20°C, effusion, Pupp et al. 1974)
7.30 × 10⁻⁶* (gas saturation-HPLC/fluo./UV, Sonnefeld et al. 1983)
2.71 × 10⁻⁴ (Yamasaki et al. 1984)
4.10 × 10⁻⁶* (selected, Howard et al. 1986)
1.51 × 10⁻³, 2.17 × 10⁻³ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P/kPa) = 12.0507 – 5925/(T/K); temp range 330–390 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 10.653 – 5461/(T/K); temp range 377–400 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
5.43 × 10⁻⁴ (supercooled liquid P_l, converted from literature P_s, Hinckley et al. 1990)
0.00107, 3.23 × 10⁻⁴ (P_l, GC by GC-RT correlation with different reference standards, Hinckley et al. 1990)
log (P/Pa) = 12.63 – 4742/(T/K) (GC-RT correlation, Hinckley et al. 1990)
5.43 × 10⁻⁴ (supercooled liquid P_l, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
(4.11–281) × 10⁻³; 2.76 × 10⁻³ (P_s, quoted exp., effusion; gas saturation, Delle Site 1997)
3.39 × 10⁻³; 5.29 × 10⁻³; 1.48 × 10⁻⁵; 2.57 × 10⁻⁵ (P_s, quoted lit., calculated; GC-RT correlation, Delle Site 1997)
5.47 × 10⁻⁴; 3.59 × 10⁻⁵ (quoted supercooled liquid P_l from Hinckley et al. 1990; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)
log (H/(Pa m³/mol)) = 9.67 – 2641/(T/K) (Passivirta et al. 1999)
log (H/(Pa m³/mol)) = 9.67 – 2641/(T/K) (Passivirta et al. 1999)
5.47 × 10⁻⁴; 3.59 × 10⁻⁵ (quoted supercooled liquid P_l from Hinckley et al. 1990; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)
ln K_{AW} = –7986.53/(T/K) + 19.124, ΔH = 66.4 kJ mol⁻¹, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)
log (K_{AW}) = 9.67 – 2641/(T/K) (Passivirta et al. 1999)

Henry’s Law Constant (Pa m³/mol at 25°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)
1.22* (gas stripping-GC; measured range 4.1–31°C, Bamford et al. 1999)
ln K_{AW} = –7986.53/(T/K) + 19.124, ΔH = 66.4 kJ mol⁻¹, measured range 4.1–31°C (gas stripping-GC, Bamford et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW} at 25°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, Yang 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 ± 0.19, 5.50 ± 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 K_{OW} = 1.238 + 1216.89/(T/K); temp range 5–55°C (temperature dependence HPLC-k′ correlation, Lei et al. 2000)

Octanol/Air Partition Coefficient, log K_{OA}:
9.50 (calculated-K_{OW}/K_{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, 4.266 (calculated-molecular connectivity indices, calculated-$K_{OW}$, Lu et al. 1999)

Sorption Partition Coefficient, log $K_{OC}$:

- 4.52 (22°C, 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 flask-HPLC/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 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of exp 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: aquatic fate rate $k = 8 \times 10^3$ h$^{-1}$ with $t_{1/2} \sim 90$ h (Callahan et al. 1979);

- half-lives predicted by one compartment model: $t_{1/2} > 1000$ h in stream, eutrophic pond or lake and oligotrophic lake (Smith et al. 1978);
- calculated $t_{1/2} = 500$ h for a river of 1-m deep with water velocity of 0.5 m/s and wind velocity of 1 m/s (Southworth 1979; quoted, Herbes et al. 1980; Hallett & Brecher 1984).

Photolysis: aquatic fate rate $k \sim 6 \times 10^{-5}$ s$^{-1}$ with $t_{1/2} = 10–50$ h (Callahan et al. 1979)

- $t_{1/2} = 20$ h in stream, $t_{1/2} = 50$ h in eutrophic pond or lake and $t_{1/2} = 10$ h in oligotrophic lake, predicted by one compartment model (Smith et al. 1978)

- direct photochemical transformation $t_{1/2}$(calc) = 0.59 h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis $t_{1/2} = 3.7$ d and 9.2 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlotzhauer 1979)

- $t_{1/2} = 0.58$ h in aquatics (quoted of EPA Report 600/7-78-074, Haque et al. 1980)

- $t_{1/2} = 0.2$ d for early day in March (Mill et al. 1981);

- $k = 1.93$ h$^{-1}$ (Zepp 1980; quoted, Mill & Mabey 1985)

- $k = 13.4 \times 10^{-5}$ s$^{-1}$ in early March with $t_{1/2} = 5$ h in pure water at 366 nm, in sunlight at 23–28°C and $k = 2.28 \times 10^{-3}$ s$^{-1}$ at 313 nm with 1% acetonitrile in filter-sterilized natural water (Mill et al. 1981);

- $k = 1.39$ h$^{-1}$ for summer midday at 40°N latitude (quoted, Mabey et al. 1982)

- $t_{1/2} = 1–3$ 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 µg/g on substrate): $t_{1/2} = 4.0$ h on silica gel, $t_{1/2} = 2.0$ h on alumina and $t_{1/2} = 38$ h on fly ash (Behymer & Hites 1985)

- first order daytime decay $k = 0.0125$ min$^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0250$ min$^{-1}$ for soot particles loading of 30–350 ng/mg (Kamens et al. 1988)

- photodegradation $k = 0.0251$ min$^{-1}$ with $t_{1/2} = 0.46$ h in ethanol-water (2:3, v/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 $k$(exptl) = 0.0251 min$^{-1}$ with the calculated $t_{1/2} = 0.46$ h and the predicted $k = 0.0245$ min$^{-1}$ calculated by QSRR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

direct photolysis $t_{1/2}(\text{obs}) = 0.94 \text{ h}$, $t_{1/2}(\text{calc}) = 0.89 \text{ h}$ predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 5.0 \times 10^{-4} \text{ s}^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: half-lives predicted by one compartment model: $t_{1/2} = 38 \text{ h}$ in stream, eutrophic pond or lake and oligotrophic lake based on peroxy radical concentration of $10^{-9} \text{ M}$ (Smith et al. 1978)

aquatic fate rate $k = 5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 38 \text{ h}$ (Callahan et al. 1979);

$k = 6400 \text{ h}$ for photosensitized oxygenation with singlet oxygen at near-surface natural water, $40^\circ \text{N}$, midday, midsummer (Zepp & Schlotzhauer 1979)

$k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for free-radical oxidation in air-saturated water (NRCC 1983)

$k = 5.0 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $2 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$\text{photooxidation } t_{1/2} = 0.801–8.01 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991);

$\text{photooxidation } t_{1/2} = 77–3850 \text{ h}$ in water, based on measured 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: 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)

$k = 3.3 \times 10^{-3} \text{ h}^{-1}$ with $t_{1/2} = 208 \text{ h}$ for mixed bacterial populations in stream sediment (NRCC 1983)

$k = 1.0 \times 10^{-4} \text{ h}^{-1}$ with $t_{1/2} = 288 \text{ d}$; $k = 4.0 \times 10^{-6} \text{ h}^{-1}$ with $t_{1/2} = 20 \text{ yr}$ for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)

$k = 0.0026 \text{ d}^{-1}$ with $t_{1/2} = 261 \text{ d}$ for Kidman sandy loam and $k = 0.0043 \text{ d}^{-1}$ with $t_{1/2} = 162 \text{ d}$ for McLarin sandy loam all at ~0.33 bar soil moisture (Park et al. 1990)

$\text{t}_{1/2}(\text{aq.aerobic}) = 2448–16320 \text{ h}$, based on aerobic soil dieaway test data at 10–30°C (Howard et al. 1991)

$\text{t}_{1/2}(\text{aq. anaerobic}) = 9792–65280 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: rate constant estimated to be $1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 669 \text{ h}^{-1}$; $k_2 = 0.144 \text{ h}^{-1}$ ($\text{Daphnia pulex}$, Southworth et al. 1978)

$\log k_1 = 2.83 \text{ h}^{-1}$; $\log k_2 = -0.84 \text{ h}^{-1}$ ($\text{Daphnia pulex}$, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

$k_1 = 138.6 \text{ mL g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0022 \text{ h}^{-1}$ (4°C, $P. h o y i$, Landrum 1988)

$k_1 = 0.72–1.4 \text{ mg g}^{-1} \text{ h}^{-1}$; $k_2 = 0.0096 \text{ h}^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

Air: $t_{1/2} = 1–3 \text{ h}$, based on estimated photolysis half-life in air (Howard et al. 1991);

$\text{t}_{1/2} = 4.20 \text{ h}$ under simulated sunlight, $t_{1/2} = 1.35 \text{ h}$ in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 2.88 \text{ h}$ in dark reaction ozone (0.2 ppm), under simulated atmospheric conditions (Katz et al. 1979)

$\text{t}_{1/2} = 0.4 \text{ h}$ for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0265 \text{ min}^{-1}$ at 1 cal cm$^{-2}$ min$^{-1}$, 10 g/m$^3$ H$_2$O and 20°C (Kamens et al. 1988).

Surface water: photolysis $t_{1/2} = 0.59 \text{ h}$ near surface water, $t_{1/2} = 3.7 \text{ d}$ and $9.2 \text{ d}$ in 5-m deep water body without and with sediment-water partitioning in full summer day, 40°N; photosensitized oxygenation $t_{1/2} = 2.6 \text{ h}$ at near surface water, 40°N, midday, midsummer (Zepp & Schlotzhauer 1979)

$\text{t}_{1/2} = 0.20 \text{ d}$ under summer sunlight (Mill & Mabey 1985);

$\text{t}_{1/2} = 1–3 \text{ h}$, based on estimated photolysis half-life in water, Howard et al. 1991); photolysis $t_{1/2} = 0.46 \text{ h}$ (reported in units of minutes) in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 4896–32640 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: The uptake clearance from sediment was $k = (0.005 \pm 0.001) \text{ g} \text{ of dry sediment} \cdot \text{g}^{-1} \text{ of organism} \cdot \text{h}^{-1}$, and the elimination rate constants $k = (0.0014 \pm 0.0006) \text{ h}^{-1}$ for amphipod, $P. h o y i$ in Lake Michigan sediments at 4°C (Landrum 1989);

desorption $t_{1/2} = 11.1 \text{ d}$ from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: $t_{1/2} = 4–6250 \text{ d}$ (Sims & Overcash 1983; quoted, Bulman et al. 1987);
t_{1/2} = 240 d for 5 mg/kg treatment and 130 d for 50 mg/kg treatment (Bulman et al. 1987); biodegradation k = 0.0026 d\(^{-1}\) with t_{1/2} = 261 d for Kidman sandy loam soil, and k = 0.0043 d\(^{-1}\) with t_{1/2} = 162 d for McLaurin sandy loam soil (Park et al. 1990); t_{1/2} ~ 2448–16320 h, based on aerobic die-away test data at 10–30°C (Howard et al. 1991); t_{1/2} > 50 d (Ryan et al. 1988).

Biota: depuration t_{1/2} = 9 d by oysters (Lee et al. 1978); elimination t_{1/2} = 4.3–17.8 d from mussel *Mytilus edulis*; t_{1/2} = 7–15.4 d from Oyster, t_{1/2} = 8.0 d from clam *Mercenaria 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

\[
S/(\mu g/kg) = a \cdot t^3 + b \cdot t^2 + c \cdot t + d \quad (1)
\]

\[
\ln x = A + \frac{B}{(T/K)} + C \cdot \ln (T/K) \quad (2)
\]

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>( S/\mu g/m^3 )</td>
<td>( t/°C )</td>
<td>( S/\mu g/m^3 )</td>
</tr>
<tr>
<td>6.9</td>
<td>0.00299</td>
<td>25</td>
<td>0.0094</td>
</tr>
<tr>
<td>10.7</td>
<td>0.00378</td>
<td>29</td>
<td>0.0122</td>
</tr>
<tr>
<td>14.3</td>
<td>0.00479</td>
<td>11.0</td>
<td>0.00361</td>
</tr>
<tr>
<td>19.3</td>
<td>0.00633</td>
<td>14.7</td>
<td>0.00558</td>
</tr>
<tr>
<td>23.1</td>
<td>0.00837</td>
<td>temp dependence eq. 1</td>
<td>18.1</td>
</tr>
<tr>
<td>29.7</td>
<td>0.0127</td>
<td>( \Delta H_{sol}/(kJ \cdot mol^{-1}) = 44.81 )</td>
<td>19.3</td>
</tr>
<tr>
<td>( a )</td>
<td>0.0003</td>
<td>( b )</td>
<td>–0.0031</td>
</tr>
<tr>
<td>( S/\mu g/kg )</td>
<td>( S/\mu g/kg )</td>
<td>29.5</td>
<td>0.0124</td>
</tr>
<tr>
<td>( \Delta H_{sol}/(kJ \cdot mol^{-1}) = 44.81 ) &amp;measured between 5–30°C &amp;</td>
<td>29.7</td>
<td>0.0127</td>
<td></td>
</tr>
<tr>
<td>( \Delta H_{sol}/(kJ \cdot mol^{-1}) = 44.81 ) &amp;measured between 5–30°C &amp;</td>
<td>1.74</td>
<td>( \Delta H_{sol}/(kJ \cdot mol^{-1}) = 44.81 ) &amp;measured between 5–30°C &amp;</td>
<td></td>
</tr>
</tbody>
</table>

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**TABLE 4.1.1.39.2**

**Reported vapor pressures of benz[a]anthracene at various temperatures and the coefficients for the vapor pressure equations**

<table>
<thead>
<tr>
<th>Equations</th>
<th>Authors</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>log ( \log P = A - \frac{B}{T/K} )</td>
<td>Kelley &amp; Rice 1964</td>
<td>effusion-electrobalance</td>
<td>10.045</td>
</tr>
<tr>
<td>log ( \log P = A - \frac{B}{C + t/°C} )</td>
<td>Murray et al. 1972</td>
<td>Knudsen effusion</td>
<td>105.21</td>
</tr>
<tr>
<td>log ( \log P = A - \frac{B}{T/K} - C \log (T/K) )</td>
<td>de Kruif 1980</td>
<td>torsion-, effusion method</td>
<td>112.62</td>
</tr>
<tr>
<td>log ( \log P = A - \frac{B}{C + T/K} )</td>
<td>Sonnefeld et al. 1983</td>
<td>generator column-HPLC</td>
<td>115.06</td>
</tr>
</tbody>
</table>

**Continued**

**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 (Continued)

<table>
<thead>
<tr>
<th></th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>effusion-electrobalance</td>
<td>Knudsen effusion</td>
<td>torsion-, effusion method</td>
<td>generator column-HPLC</td>
</tr>
<tr>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>t/°C P/Pa</td>
<td>eq. 1 P/mmHg</td>
</tr>
<tr>
<td>eq. 1</td>
<td>13.68</td>
<td>9.684</td>
<td>A</td>
<td>9.684</td>
</tr>
<tr>
<td>A</td>
<td>6250</td>
<td>4246.51</td>
<td>B</td>
<td>4246.51</td>
</tr>
<tr>
<td>for temp range 60–120°C</td>
<td></td>
<td></td>
<td></td>
<td>ΔHsub/(kJ mol⁻¹) = 51.83</td>
</tr>
</tbody>
</table>

for temp range 10–50°C

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

\[
\ln K_{AW} = A - B/(T/K) \quad (1) \\
\ln (1/K_{AW}) = A - B/(T/K) \quad (2) \\
\ln (k_h/\text{atm}) = A - B/(T/K) \quad (3) \\
\ln \left( \frac{H/\text{Pa m}^3/\text{mol}}{} \right) = A - B/(T/K) \quad (4) \\
K_{AW} = A - B/(T/K) + C/(T/K)^2 \quad (5)
\]

Bamford et al. 1999

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>average</td>
</tr>
<tr>
<td>4.1</td>
<td>0.10, 0.22</td>
<td>0.15</td>
</tr>
<tr>
<td>11.0</td>
<td>0.24, 0.41</td>
<td>0.31</td>
</tr>
<tr>
<td>18.0</td>
<td>0.50, 0.79</td>
<td>0.63</td>
</tr>
<tr>
<td>25.0</td>
<td>0.91, 1.64</td>
<td>1.22</td>
</tr>
<tr>
<td>31.0</td>
<td>1.43, 3.13</td>
<td>2.11</td>
</tr>
</tbody>
</table>

\ln K_{AW} = A - B/(T/K)

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TABLE 4.1.1.39.3 (Continued)

Bamford et al. 1999

gas stripping-GC/MS

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/(Pa m³/mol)</th>
<th>H/(Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>19.124</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>7986.5</td>
<td></td>
</tr>
</tbody>
</table>

enthalpy, entropy change:

\[ \Delta H/(kJ\cdot mol^{-1}) = 66.4 \pm 6.9 \]

\[ \Delta S/(J\cdot K^{-1}\cdot mol^{-1}) = 159 \]

at 25°C

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, benzo[**e**]acephenanthrylene, B[**b**]F
Chemical Name: 2,3-benzofluoranthene
CAS Registry No: 205-99-2
Molecular Formula: C_{20}H_{12}
Molecular Weight: 252.309

**Melting Point (°C):**
168 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)

**Boiling Point (°C):**
481 (Bjørseth 1983)

**Density (g/cm³ at 20°C):**

**Molar Volume (cm³/mol):**
222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
268.9 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**
56.5 (Passivirta et al. 1999)

**Entropy of Fusion, ΔS_{fus} (J/mol K):**

**Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:** 0.0395 (mp at 168°C)

**Water Solubility (g/m³ or mg/L at 25°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 [S_L/(mol/L)] = – 0.351 – 1303/(T/K) (supercooled liquid, Passivirta et al. 1999)

**Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):**
6.67 × 10⁻⁵ (20°C, estimated, Callahan et al. 1979)
2.12 × 10⁻⁵ (Yamasaki et al. 1984)
5.0 × 10⁻⁶; 1.30 × 10⁻⁶ (quoted solid Pᵥ from Mackay et al. 1992; converted to supercooled liquid Pᵥ with fugacity ratio F, Passivirta et al. 1999)
log (Pᵥ/Pa) = 12.43 – 5880/(T/K) (solid, Passivirta et al. 1999)
log (Pᵥ/Pa) = 9.48 – 4578/(T/K) (supercooled liquid, Passivirta et al. 1999)
7.55 × 10⁻⁶ (supercooled liquid Pᵥ, calibrated GC-RT correlation, Lei et al. 2002)
log (Pᵥ/Pa) = –4682/(T/K) + 10.58, ΔH_{vap.} = –89.7 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)

**Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations.):**
0.051 (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)
log [H/(Pa m³/mol)] = 9.83 – 3274/(T/K) (Passivirta et al. 1999)
0.0485 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 2.955 – 2245/(T/K), (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

**Octanol/Water Partition Coefficient, log K_{ow}:**
5.78 (HPLC-RT correlation, Wang et al. 1986)
5.78 (recommended, Sangster 1989, 1993)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF:

- 5.15 (microorganisms-water, Mabey et al. 1982)
- 4.00 ($Daphnia magna$, Newsted & Giesy 1987)
- 0.959, 0.230 ($Polychaete sp, Capitella capitata$, Bayona et al. 1991)

Sorption Partition Coefficient, log $K_{OC}$ at 25°C or as indicated:

- 6.182; 6.00, 6.18 (sediment: concn ratio $C_{sed}/C_{aq}$; concn-based coeff., areal-based coeff. of flux studies of sediment/water boundary layer, Helmstetter & Alden 1994)
- 5.45 (log $K_{DOC}$ - Aldrich humic acid, RP-HPLC, Ozretich et al. 1995)
- 5.7 (10°C), 6.55, 6.61 (20°C), 6.26 (35°C), 6.44, 6.45 (45°C) (log $K_{DOC}$, dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
- 6.20 (20°C, log $K_{DOC}$, 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 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of exp 1,2,3, solvophobic approach, Krauss & Wilcke 2001, for benzo[$b+j+k$]fluoranthenes)

Environmental Fate Rate Constants, k or Half-Lives, $t_1/2$:

Volutilization:

Photolysis: atmospheric and aqueous $t_1/2 = 8.7–720$ h, based on measured rate of photolysis in heptane irradiated with light > 290 nm (Howard et al. 1991);

first order daytime decay rate constants: $k = 0.0065$ min$^{-1}$ for 1000–2000 ng/mg soot particles loading and $k = 0.0090$ min$^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988);

$\text{t}_{1/2}(\text{obs.}) = 4.31$ h, $\text{t}_{1/2}(\text{calc}) = 1.49$ h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)

Photodegradation $k = 3 \times 10^{-5}$ s$^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002).

Oxidation: rate constant $k = 4 \times 10^7$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 5 \times 10^3$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 1.43–14.3$ 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 $t_{1/2} = 8640–14640$ h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$k = 0.0024$ d$^{-1}$ with $t_{1/2} = 294$ d for Kidman sandy loam and $k = 0.0033$ d$^{-1}$ with $t_{1/2} = 211$ d for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990);

$\text{t}_{1/2}(\text{aq. anaerobic}) = 34560–58560$ h, based on estimated unacclimated aqueous aerobic degradation half-life (Howard et al. 1991).

Biotransformation: estimated to be $3 \times 10^{-12}$ mL cell$^{-1}$ h$^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

$k_1 = 0.11–0.38$ mg g$^{-1}$ h$^{-1}$; $k_2 = 0.0029$ h$^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Sorption-Desorption Rate constants: desorption rate constant $k = 0.016$ d$^{-1}$ with $t_{1/2} = 42.4$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Half-Lives in the Environment:

Air: $t_{1/2} = 1.43–14.3$ h, based on estimated photooxidation half-life in air (Howard et al. 1991)

half-lives under simulated atmospheric conditions: simulated sunlight – $t_{1/2} = 8.70$ h, simulated sunlight + ozone (0.2 ppm) $t_{1/2} = 4.20$ h, dark reaction ozone (0.2 ppm) $t_{1/2} = 52.70$ h (Katz et al. 1979; quoted, Bjørseth & Oluften 1983);

$t_{1/2} = 1.3$ h for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0091$ min$^{-1}$ at 1 cal cm$^{-2}$ min$^{-1}$, 10 g/m$^3$ H$_2$O and 20°C (Kamens et al. 1988).

Surface water: $t_{1/2} = 8.7–720$ h, based on estimated aqueous photolysis half-life (Lane & Katz 1977; Muel & Saguem 1985; quoted, Howard et al. 1991).
Groundwater: \( t_{1/2} = 17280–29280 \) h, based on estimated unacclimatized aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: desorption \( t_{1/2} = 42.4 \) d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).

Soil: biodegradation rate constant \( k = 0.0024 \) d\(^{-1}\) with \( t_{1/2} = 294 \) d for Kidman sandy loam soil, and \( k = 0.0033 \) d\(^{-1}\) with \( t_{1/2} = 211 \) d for McLaurin sandy loam soil (Park et al. 1990);

\( t_{1/2} = 8640–14640 \) h, based on aerobic die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

\( t_{1/2} = 42 \) wk, 9.0 yr (quoted, Luddington soil, Wild et al. 1991).

Biota: elimination \( t_{1/2} = 5.7–16.9 \) d from mussel *Mytilus edulis*; \( t_{1/2} = 7.7 \) d from Oyster (isomer unspecified),

\( t_{1/2} = 3.9 \) d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).
4.1.1.41  **Benzo[j]fluoranthene**

![Chemical structure image]

**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:** C_{20}H_{12}  
**Molecular Weight:** 252.309

**Melting Point (°C):**  
166 (Bjørseth 1983; Pearlman et al. 1984; Lide 2003)

**Boiling Point (°C):**  
480 (Bjørseth 1983)

**Density (g/cm³ at 20°C):**  
222.8 (Ruelle & Kesselring 1997)  
268.9 (calculated-Le Bas method at normal boiling point)

**Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):**  

**Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):**  

**Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F:** 0.0414 (mp at 166°C)

**Water Solubility (g/m³ or mg/L at 25°C):**  
0.0025 (generator column-HPLC/fluorescence, Wise et al. 1981)  
0.0025 (average lit. value, Pearlman et al. 1984)

**Vapor Pressure (Pa at 25°C):**

**Henry’s Law Constant (Pa m³/mol):**

**Octanol/Water Partition Coefficient, log K_{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 K_{OA}:**

**Bioconcentration Factor, log BCF:**  
0.914; –0.222 (Polychaete sp, Capitella capitata, Bayona et al. 1991)

**Sorption Partition Coefficient, log K_{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 (20°C, 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, \( t_{1/2} \):**

**Half-Lives in the Environment:**  
Biota: elimination \( t_{1/2} = 7.7 \) d from Oyster (isomer unspecified), \( t_{1/2} = 3.9 \) 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: C_{20}H_{12}
Molecular Weight: 252.309
Melting Point (°C):
217 (Weast 1977; Bjørseth 1983; Stephenson & Malanowski 1987; Lide 2003)
Boiling Point (°C):
480 (Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 20°C): 222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
268.9 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
56.6 (Passivirta et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0126 (mp at 217°C)
0.008 (generator column-HPLC/UV, Wise et al. 1981)
0.0081 (average lit. value, Pearlman et al. 1984)
0.00109 (generator column-HPLC/fluorescence, De Maagd et al. 1998)
Water Solubility (g/m³ or mg/L at 25°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)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.28 × 10⁻⁸ (20°C, Radding et al. 1976)
6.70 × 10⁻⁵ (20°C, Mabey et al. 1982)
2.07 × 10⁻⁵ (Yamasaki et al. 1984)
5.20 × 10⁻⁴, 4.93 × 10⁻⁶ (20°C, lit. mean solid P_s, supercooled liquid value P_L, Bidleman & Foreman 1987)
1.29 × 10⁻⁷ (extrapolated, Antoine eq., Stephenson & Malanowski 1987)
log (P_s/kPa) = 12.8907 – 6792/(T/K); temp range 363–430 K (Antoine eq., Stephenson & Malanowski 1987)
2.09 × 10⁻⁵ (supercooled liquid P_L, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
log (P_s/(mol/L)) = –0.351 – 1448/(T/K) (supercooled liquid, Passivirta et al. 1999)
log (P_L/Pa) = 9.48 – 4427/(T/K) (supercooled liquid, Passivirta et al. 1999)
8.96 × 10⁻⁶ (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)
log (P_L/Pa) = –4623/(T/K) + 10.46; ΔH_{vap.} = –88.5 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol at 25°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 (15°C, calculated, Baker & Eisenreich 1990)
0.043* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)
log (H/(Pa m³/mol)) = 9.83 – 2979/(T/K) (Passivirta et al. 1999)
0.0422 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 3.498 – 2421/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Water Partition Coefficient, log $K_{ow}$:
- 6.84 (calculated-fragment const., Callahan et al. 1979)
- 6.06 (calculated-f const., Mabey et al. 1982)
- 6.44 (calculated-MCI $\chi$ as per Rekker & De Kort 1979)
- 6.40 (Bayona et al. 1991)
- 6.50 (calculated-S and mp, Capel et al. 1991)
- 7.20 (calculated-$K_{oc}$, 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 $K_{oa}$:
- 11.19 (calculated, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
- 5.15 (microorganisms-water, calculated from $K_{ow}$, Mabey et al. 1982)
- 4.12 ($Daphnia magna$, Newsted & Giesy 1987)

Sorption Partition Coefficient, log $K_{oc}$ at 25°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 (10°C), 6.74, 6.89 (20°C), 6.46 (35°C), 6.44, 6.45 (45°C) (log $K_{DPC}$ - dissolved organic material from lake, gas-purge technique- HPLC/fluorescence, Lüers & ten Hulscher 1996)
- 6.30 (20°C, log $K_{Poc}$ - 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 flask-HPLC/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[\textit{b} + \textit{j} + \textit{k}]fluoranthenes)
- 5.91; 6.50, 6.26, 6.68 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1, 2, 3-solvophobic approach, Krauss & Wilcke 2001, for benzo[\textit{b} + \textit{j} + \textit{k}]fluoranthenes)

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:

Volatilization:
- Photolysis: atmospheric and aqueous photolysis $t_{v} = 3.8–499$ 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: $k = 0.0047$ min$^{-1}$ for soot particles loading of 1000–2000 ng/mg and $k = 0.0013$ min$^{-1}$ with 30–350 ng/mg loading (Kamens et al. 1988);
- direct photolysis $t_{v}$(obs) = 0.88 h, $t_{v}$(calc) = 0.80 h predicted by QSPR in atmospheric aerosol (Chen et al. 2001)
- Photodegradation $k = 3 \times 10^{-5}$ s$^{-1}$ in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

Oxidation: rate constant $k = 4 \times 10^{7}$ M$^{-1}$ h$^{-1}$ for singlet oxygen and $k = 5 \times 10^{9}$ M$^{-1}$ h$^{-1}$ for peroxy radical (Mabey et al. 1982);
- photooxidation $t_{i} = 1.1–11$ 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 $t_{i} = 21840–51360$ h, based on aerobic soil die-away test data (Howard et al. 1991);
- $t_{i}$(aq. anaerobic) = 87360–205440 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
Biotransformation: estimated to be $3 \times 10^{-12}$ mL cell$^{-1}$ h$^{-1}$ for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

- Air: $t_{1/2} = 1.1–11$ h, based on estimated photooxidation half-life in air (Howard et al. 1991);
- $t_{1/2} = 14.10$ h in simulated sunlight; $t_{1/2} = 3.90$ h in simulated sunlight + ozone (0.2 ppm), $t_{1/2} = 34.90$ h in dark reaction ozone (0.2 ppm) u) under simulated atmospheric conditions (Katz et al. 1979);
- $t_{1/2} = 0.8$ h for adsorption on soot particles in an outdoor Teflon chamber with an estimated rate constant $k = 0.0138$ min$^{-1}$ at 1 cal cm$^{-2}$ min$^{-1}$ and 10 g/m$^3$ H$_2$O at 20°C (Kamens et al. 1988).
- Surface water: $t_{1/2} = 3.8–499$ h, based on photolysis half-life in water (Howard et al. 1991).
- Groundwater: $t_{1/2} = 42680–102720$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).
- Sediment: desorption $t_{1/2} = 23.2$ d from sediment under conditions mimicking marine disposal (Zhang et al. 2000).
- Soil: $t_{1/2} = 21840–51360$ h, based on aerobic soil die-away test data Howard et al. 1991);
- $t_{1/2} > 50$ d (Ryan et al. 1988);
- mean $t_{1/2} = 8.7$ yr for Luddington soil (Wild et al. 1991).
- Biota: elimination $t_{1/2} = 11.9$ d from mussel *Mytilus edulis*; $t_{1/2} = 7.7$ d from Oyster (isomer unspecified), $t_{1/2} = 3.9$ d from clam *Mercenaria mercenaria* (isomer unspecified) (quoted, Meador et al. 1995).

### TABLE 4.1.42.1
Reported Henry’s law constants of benzo[k]fluoranthene at various temperatures and temperature dependence equations

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>H/(Pa m$^3$/mol)</th>
<th>$\ln K_{AW}$ = $A - B/(T/K)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>0.022</td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>0.043</td>
<td></td>
</tr>
<tr>
<td>35.0</td>
<td>0.107</td>
<td></td>
</tr>
<tr>
<td>40.1</td>
<td>0.138</td>
<td></td>
</tr>
<tr>
<td>45.0</td>
<td>0.198</td>
<td></td>
</tr>
<tr>
<td>55.0</td>
<td>0.403</td>
<td></td>
</tr>
</tbody>
</table>

$K_{AW} = A - B/(T/K) + C/(T/K)^2$  

$\ln K_{AW} = -\Delta H_{vol}/RT + \Delta S_{vol}/R$  

$R = 8.314$ Pa m$^3$ mol$^{-1}$ K$^{-1}$  

$\Delta S_{vol} = 16.41$  

$\Delta H_{vol} = 5893.7$  

**enthalpy of volatilization:**  
$\Delta H_{vol}/(kJ/mol) = 49 \pm 1.9$  

**entropy of volatilization:**  
$T\Delta S_{vol}/(kJ/mol) = 40 \pm 4$  

* at 20°C
**FIGURE 4.1.142.1** Logarithm of Henry's law constant versus reciprocal temperature for benzo[k]fluoranthene.
### 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:** C_{20}H_{12}  
**Molecular Weight:** 252.309  
**Melting Point (°C):**  
181.1  
(Stephenson & Malanowski 1987; Dean 1992)  
**Boiling Point (°C):**  
495  
(Stephenson & Malanowski 1987; Dean 1992)  
**Density (g/cm³ at 20°C):**  
**Molar Volume (cm³/mol):**  
222.8  
(Ruelle & Kesselring 1997; Passivirta et al. 1999)  
262.9  
(calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, ΔH_{fus} (kJ/mol):**  
17.324  
(Ruelle & Kesselring 1997)  
8.49, 17.32; 25.61 (117.05, 181.05°C; total phase change enthalpy, Chickos et al. 1999)  
**Entropy of Fusion, ΔS_{fus} (J/mol K):**  
38.5  
(differential scanning calorimetry, Hinckley et al. 1990)  
21.77, 38.13 (117.05, 181.05°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°C (assuming ΔS_{fus} = 56 J/mol K), F:**  
0.0294  
(mp at 181.1°C)  
0.0903  
(calculated, Passivirta et al. 1999)  
**Water Solubility (g/m³ or mg/L at 25°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  
(27°C, nephelometry, Davis et al. 1942)  
0.0043  
(shake flask-UV/fluorescence, Barone et al. 1967)  
0.0061  
(average, Barone et al. 1967)  
0.0005  
(20°C, 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°C, May et al. 1983)  
0.00158*  
(generator column-spectrofluorimetry, measured range 10–30°C, Velapoldi et al. 1983)  
0.0038  
(selected value, Pearlman et al. 1984)  
0.00154*  
(generator column-HPLC/UV, measured 8.0–25.0°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 ± 0.00023; 0.0038, 0.0018 ± 0.0003 (shake flask-SPME (solid-phase micro-extraction)-GC; quoted lit. values; Paschke et al. 1999)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

log $S_L$ (mol/L) = −1.310 − 906.6/(T/K) (supercooled liquid, Passivirta et al. 1999)

$\ln x = −2.59638 − 6046.87/(T/K)$; temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

- $7.32 \times 10^{-7}$ (effusion method, extrapolated, Murray et al. 1974)
- $\log(P/mmHg) = 9.601 − 6181/(T/K)$; temp range 358–431 K (Knudsen effusion method, Murray et al. 1974)
- $1.12 \times 10^4, 1.50 \times 10^5$ ($P_{GC}$, GC-RT correlation with different GC columns, Bidleman 1984)
- $2.35 \times 10^{-3}$ (supercooled liquid $P_L$, converted from literature $P_S$ with $\Delta S_{ fus}$ Bidleman 1984)
- $1.22 \times 10^{-3}$ (Yamasaki et al. 1984)
- $3.2 \times 10^{-7}, 1.23 \times 10^{-5}$ (lit. mean, supercooled liq. value, Bidleman & Foreman 1987)
- $7.51 \times 10^{-2}$ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P/kPa) = 11.6067 − 6181/(T/K)$; temp range 358–431 K (Antoine eq., Stephenson & Malanowski 1987)
- $1.17 \times 10^{-3}$ (supercooled liquid $P_L$, calculated from Yamasaki et al 1984, Finizio et al. 1997)
- $2.35 \times 10^{-5}, 7.28 \times 10^{-6}$ (supercooled liquid $P_L$, converted from literature $P_S$ with different $\Delta S_{ fus}$ Hinckley et al. 1990)
- $1.12 \times 10^{-4}, 7.24 \times 10^{-5}$ (PGC, GC-RT correlation with different reference standards, Hinckley et al. 1990)
- $1.54 \times 10^{-6}; 1.39 \times 10^{-6}$ (quoted supercooled liquid $P_L$ from Hinckley et al. 1990; converted to solid $P_S$ with fugacity ratio F, Passivirta et al. 1999)
- $\log(H/(Pa m^3/mol)) = 12.17 − 5371/(T/K)$ (solid, Passivirta et al. 1999)
- $\log(K_{AW}) = 1.732 − 1927/(T/K)$ (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Henry’s Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- $0.009$ (15°C, calculated, Baker & Eisenreich 1990)
- $0.0079$ (10°C, estimated, McLachlan et al. 1990)
- $0.034^*$ (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)
- $0.074$ (wetted wall column-GC, Altschuh et al. 1999)
- $\log[H/(Pa m^3/mol)] = 12.02 − 3558/(T/K)$ (Passivirta et al. 1999)
- $0.035$ (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
- $\log K_{OW}$:
  - 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 ± 0.1 (25°C, shake flask-concentration ratio/UV spec.; shake flask-HPLC/UV; exp. 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)
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6.02 ± 0.19, 6.14 ± 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 K_{OA}:
10.80 (calculated-K_{OW}/K_{AW}, Wania & Mackay 1996)
10.77 (calculated, Finizio et al. 1997)

Bioconcentration Factor, log BCF:
1.09; 2.22; 3.45 (steady-state, bluegills; midge larva; periphyton, Leversee et al. 1981)
4.74 (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 (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 (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 (Daphnia magna, Newsted & Giesy 1987)
4.61, 3.86, 3.87 (4°C, 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 K_{POC} at 25°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 (10°C), 6.46, 6.60 (20°C), 6.14 (35°C), 6.07, 6.09 (45°C) (log K_{POC} - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.30 (20°C, log K_{POC} - 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 (pH 5, 6.5, 8, humic acid from sediments of River Arno, De Paolis & Kokkonen 1997)
4.81, 4.87, 4.49 (pH 5, 6.5, 8, fulvic acid from sediments of River Arno, De Paolis & Kokkonen 1997)
5.54, 5.59, 5.37 (pH 5, 6.5, 8, HA + FA extracted from sediments of River Arno, De Paolis & Kokkonen 1997)
5.51, 5.74, 5.68 (pH 5, 6.5, 8, HA extracted from sediments of Tyrenhian Sea, De Paolis & Kokkonen 1997)
4.93, 4.84, 4.85 (pH 5, 6.5, 8, FA extracted from sediments of Tyrenhian Sea, De Paolis & Kokkonen 1997)
5.66, 5.46, 5.60 (pH 5, 6.5, 8, HA + FA from sediments of Tyrenhian Sea, De Paolis & Kokkonen 1997)
5.22, 5.46, 5.60 (pH 5, 6.5, 8, HA extracted from water of River Arno, De Paolis & Kokkonen 1997)
4.67, 4.80, 4.45 (pH 5, 6.5, 8, FA extracted from water of River Arno, De Paolis & Kokkonen 1997)
5.21, 5.29, 5.18 (pH 5, 6.5, 8, HA + FA extracted from water of River Arno, De Paolis & Kokkonen 1997)
4.62, 4.52, 4.61 (pH 5, 6.5, 8, FA extracted from water of Tyrenhian Sea, De Paolis & Kokkonen 1997)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

5.99 (5.92–6.04), 5.53 (5.43–5.61) (sediments: Lake Oostvaardersplassen, Lake Ketelmeer, shake flask-HPLC/UV, de Maag 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 (log K_{DOC}: 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)
5.3 (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 (20°C, 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, t½:

Volatilization: aquatic fate rate of 300 h–1 with t½ = 22 h (Callahan et al. 1979);
half-lives predicted by one compartment model: t½ = 140 h in river water, t½ = 350 h in eutrophic pond, t½ = 700 h in eutrophic lake and oligotrophic lake (Smith et al. 1978);
calculated t½ = 1500 h for a river of 1-m deep with water velocity of 0.5 m s–1 and wind velocity of 1 m/s (Southworth 1979; Herbes et al. 1980);
sublimation rate constant from glass surface of < 1 × 10–5 s–1 was measured at 24°C at an airflow rate of 3 L/min (Cope & Kalkwarf 1987).

Photolysis: photolysis t½ = 2 h in methanol solution when irradiated at 254 nm (Lu et al. 1977);
k = 0.58 h–1 for winter at midday at 40°N latitude (Smith et al. 1978);
direct photochemical transformation t½(calc) = 0.54 h, computed near-surface water, latitude 40°N, midday, midsummer and photolysis t½ = 3.2 d and 13 d in 5-m deep inland water body without and with sediment-water partitioning, respectively, to top cm of bottom sediment over full summer day, 40°N (Zepp & Schlottzhauer 1979)
k(aq.) = 2.8 × 10–4 s–1 with t½ = 1–2 h (Callahan et al. 1979)
photolytic t½(aq) = 0.53 h (quoted of EPA Report 600/7-78-074, Haque et al. 1980)
k = 1.30 h–1 (Zepp 1980)

half-lives predicted by one compartment model: t½ = 3.0 h in river water based on the photolysis rates estimated for summer sunlight, t½ = 7.5 h in eutrophic pond or eutrophic lake, and t½ = 1.5 h in oligotrophic lake (Smith et al. 1978; quoted, Harris 1982)
k = 2.8 × 10–4 s–1 with t½ = 1–2 h (Callahan et al., 1979)
calculated direct photolysis k = 3.86 × 10–5 s–1 in late January with t½ = 0.69 h in pure water at 366 nm and in sunlight at 23–28°C and k = 1.05 × 10–5 s–1 in mid-December with t½ = 1.1 h at 313 nm with 1–20% acetonitrile as cosolvent in filter-sterilized natural water (Mill et al. 1981)
t½ = 0.37–1.1 h, based on estimated photolysis half-life in air (Howard et al. 1991)
sunlight photolysis t½ = 0.045 d for mid-December (Mill & Mabey 1985)

half-lives on different atmospheric particulate substrates (approx. 25 µg/g on substrate): t½ = 4.7 h on silica gel, t½ = 1.4 h on alumina and t½ = 31 h on fly ash (Behymer & Hites 1985)
ozonation rate constant k < 6.1 × 10–4 m/s was measured at 24°C with [O₃] = 0.16 ppm and light intensity of 1.3 kW/m² (Cope & Kalkwarf 1987)
first order daytime decay k = 0.0090 min–1 for soot particles loading of 1000–2000 ng/mg and k = 0.0211 min–1 with 30–350 ng/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 k = 0.0322 min–1 and t½ = 0.35 h in ethanol-water (3:7, v/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 k(expt) = 0.0322 min–1 with the calculated t½ = 0.35 h and the predicted t½ = 0.0416 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 t½(obs) = 0.50 h, t½(calc) = 0.57 h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001)
photochemical degradation under atmospheric conditions: \(k = (1.18 \pm 0.50) \times 10^{-2} \text{ s}^{-1}\) and \(t_{1/2} = (1.63 \pm 0.48)\text{ h}\) in diesel particulate matter, rate constant \(k = (3.09 \pm 0.23) \times 10^{-5} \text{ s}^{-1}\) and \(t_{1/2} = (6.22 \pm 0.51)\text{ h}\) in diesel particulate matter/soil mixture, and \(t_{1/2} = 0.35\) to \(1.62\text{ h}\) in various soil components using a 900-W photo-irradiator as light source; rate constant \(k = (2.92 \pm 0.23) \times 10^{-5} \text{ s}^{-1}\) and \(t_{1/2} = (6.59 \pm 0.49)\text{ h}\) in diesel particulate matter using a 300-W light source (Matsuzawa et al. 2001).

Photodegradation \(k = 2.1 \times 10^{-3} \text{ s}^{-1}\) in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002).

Oxidation: rate constant \(k\), for gas-phase second order rate constants, \(k_{\text{OH}}\) for reaction with OH radical, \(k_{\text{NO}_3}\) with NO\(_3\) radical and \(k_{\text{O}_3}\) with \(\text{O}_3\) or as indicated, *data at other temperatures see reference:

- \(t_{1/2} > 340 \text{ h}\) in river water, eutrophic pond or lake and oligotrophic lake, half-lives predicted by one compartment model (Smith et al. 1978)
- \(k = 5 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}\), with half-life of 96 h (Callahan et al. 1979)
- \(t_{1/2} = 1500 \text{ h}\) for photosensitized oxygenation with singlet oxygen at near-surface natural water, 40°N, midday, summer (Zepp & Schlotzhauer 1979)
- \(k = 0.62 \times 10^4 \text{ dm}^{-3} \text{ mol}^{-1} \text{ s}^{-1}\) for the reaction with \(\text{O}_3\) in water at pH 7 and 25°C with \(t_{1/2} = 1.0 \text{ s}\) in presence of \(10^{-4} \text{ M}\) of ozone at pH 7 (Butković et al. 1983)
- \(k(\text{aq.}) = 3.6 \times 10^4 \text{ h}^{-1}\) with \(t_{1/2} = 0.5 \text{ h}\) under natural sunlight conditions; \(k(\text{aq.}) = 1.9 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}\) with \(t_{1/2} = 4.3 \text{ d}\) free-radicals oxidation in air-saturated water (NRCC 1983)
- \(k_{\text{NO}_3,(\text{calc})} = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}\) with hydroxyl radical in aqueous solutions (Haag & Yao 1992).


Biodegradation:

- \(k = 0.2–0.9 \text{ µmol}^{-1} \text{ mg}^{-1}\) for bacterial protein (Callahan et al. 1979)
- \(k = 3.4 \times 10^{-1} \text{ h}^{-1}\) with \(t_{1/2} = 83 \text{ h}\) for mixed bacterial populations in stream sediment (NRCC 1983)
- \(k < 3 \times 10^{-5} \text{ h}^{-1}\) with \(t_{1/2} > 2.5 \text{ yr}\); \(k < 3 \times 10^{-5} \text{ h}^{-1}\) with \(t_{1/2} > 2.5 \text{ yr}\) for mixed bacterial populations in oil-contaminated and pristine stream sediments (NRCC 1983)
- \(k = 3.5 \times 10^{-3} \text{ h}^{-1}\) estimated in water and soil (Ryan & Cohen 1986)
- \(t_{1/2(\text{aerobic})} = 57 \text{ d} \pm 1.45 \text{ yr}\) at 10–30°C, soil die-away test (Coover & Sims 1987; quoted, Howard et al. 1991); \(k = 0.0022 \text{ d}^{-1}\) with \(t_{1/2} = 309 \text{ d}\) for Kidman sandy loam and \(k = 0.0030 \text{ d}^{-1}\) with \(t_{1/2} = 229 \text{ d}\) for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990)
- \(t_{1/2(\text{anaerobic})} = 228 \text{ d} \pm 5.8 \text{ yr}\) based on estimated unacclimated aqueous aerobic biodegradation half-life (Coover & Sims 1987; quoted, Howard et al. 1991).

Biotransformation: estimated to be \(3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1}\) for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake \((k_1)\) and Elimination \((k_2)\) Rate Constants:

- \(k_1 = 49 \text{ h}^{-1}; k_2 = 0.010 \text{ h}^{-1}\) (bluegill sunfish, Spacie et al. 1983)
- \(k_1 = 131.1 \text{ mL g}^{-1} \text{ h}^{-1}; k_2 = 0.0033 \text{ h}^{-1}\) (4°C, \(P. h o y i), \text{ Landrum 1988}\)
- \(k_1 = 81.3 \text{ h}^{-1}; k_2 = 0.014 \text{ h}^{-1}\) (10–20°C, \(H. \text{ limbata}, \text{ Landrum & Poore 1988}\))
- \(k_1 = 16.8 \text{ h}^{-1}; k_2 = 0.0016 \text{ h}^{-1}\) (4°C, \(P. h o y i), \text{ Landrum & Poore 1988}\)
- \(k_1 = 87.8 \text{ h}^{-1}; k_2 = 0.012 \text{ h}^{-1}\) (4°C, \(S. \text{ heringianus}, \text{ quoted, Landrum & Poore 1988}\))
- \(k_1 = 112.0 \text{ h}^{-1}; k_2 = 0.013 \text{ h}^{-1}\) (4°C, \(Mysis \text{ relicta}, \text{ quoted, Landrum & Poore 1988}\))
- \(k_1 = 75.9 \text{ mL g}^{-1} \text{ h}^{-1}\) (\(\text{Pontoporeia hoyi}\), Evans & Landrum 1989)
- \(k_1 = 39.9 \text{ mL g}^{-1} \text{ h}^{-1}\) (\(\text{Mysis relicta}\), Evans & Landrum 1989)
- \(k_1 = 0.0047 \text{ h}^{-1}\) (\(\text{Mysis}\), Evans & Landrum 1989)
- \(k_1 = 0.11–0.36 \text{ mg g}^{-1} \text{ h}^{-1}\); \(k_2 = 0.0032 \text{ h}^{-1}\) (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

- \(t_{1/2} = 0.37–1.1 \text{ h}\) based on estimated photolysis half-life (Lyman et al. 1982; quoted, Howard et al. 1991);
- half-lives under simulated atmospheric conditions: \(t_{1/2} = 5.30 \text{ h}\) in simulated sunlight, \(t_{1/2} = 0.58 \text{ h}\) in simulated sunlight + ozone (0.2 ppm), \(t_{1/2} = 0.62 \text{ h}\) in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);
- \(t_{1/2} = 14 \text{ h}\) with a steady-state concn of tropospheric ozone of \(2 \times 10^{-9} \text{ M}\) in clean air (Butković et al. 1983);
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

photooxidation $t_{1/2} = 0.428 - 4.28$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991); $t_{1/2} = 0.5$ h for adsorption on soot particles in an outdoor Teflon chamber with an estimated $k = 0.0234$ min$^{-1}$ at 1 cal cm$^{-2}$ min$^{-1}$, 10 g m$^{-3}$ H$_2$O and 20°C (Kamens et al. 1988).

Surface Water: $t_{1/2} = 2$ h in methanol solution irradiated at 254 nm (Lu et al. 1977); half-lives predicted by one compartment model: $t_{1/2} > 340$ 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 $t_{1/2} = 0.54$ h at latitude 40°N, midday, midsummer, and direct photolysis, $t_{1/2} = 3.2$ d (no sediment-water partitioning) and $t_{1/2} = 13$ d (with sediment-water partitioning) in a 5-m deep inland water body (Zepp & Schlotzhauer 1979); $t_{1/2} = 0.37 - 1.1$ h, based on photolysis half-life in water (Lyman et al. 1982; quoted, Howard et al. 1991); $t_{1/2} = 1.0$ s in presence of $10^{-4}$ M of ozone at pH 7 (Butkovic’ et al. 1983); $t_{1/2} = 4.3$ d free-radical oxidation in air-saturated water (NRCC 1983); $t_{1/2} = 0.045$ d under mid-December sunlight (Mill & Mabey 1985); photolysis $t_{1/2} = 0.35$ h in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996).

Groundwater: $t_{1/2} = 2736 - 25440$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: uptake clearance from sediment $k = (0.0023 \pm 0.001) g$ of dry sediment·g$^{-1}$ of organism·h$^{-1}$ for amphipod, $P. hoyi$ in Lake Michigan sediments at 4°C (Landrum 1989); desorption $t_{1/2} = 19.5$ 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); $t_{1/2} = 347$ d for 5 mg/kg treatment and $t_{1/2} = 218$ d for 50 mg/kg treatment (Bulman et al. 1987); biodegradation $k = 0.002$ d$^{-1}$ with $t_{1/2} = 309$ d for Kidman sandy loam soils and $k = 0.003$ d$^{-1}$ with $t_{1/2} = 229$ d for McLaurin sandy loam soils (Park et al. 1990); $t_{1/2} = 1368 - 12720$ h, based on aerobic soil dieaway test data at 10–30°C (Groenewegen & Stolp 1976; Coover & Sims 1987; quoted, Howard et al. 1991); $t_{1/2} > 50$ d (Ryan et al. 1988); $t_{1/2} = 0.3$ to > 300 wk, 8.2 yr (literature, Luddington soil, Wild et al. 1991).

Biota: depuration $t_{1/2} = 18$ d by oysters (Lee et al. 1978; quoted, Verschueren 1983); $t_{1/2} = 67$ h in bluegill sunfish (Spacie et al. 1983); depuration $t_{1/2} = 52$ h in $s. heringianus$ (Frank et al. 1986); calculated half-lives in different tissues of sea bass: $t_{1/2} = 12.4$ d for fat, $t_{1/2} = 6.5$ d for kidney, $t_{1/2} = 5.1$ d for kidney, $t_{1/2} = 5.1$ d for intestine, $t_{1/2} = 4.8$ d for gallbladder, $t_{1/2} = 4.5$ d for spleen, $t_{1/2} = 2.9$ d for muscle, $t_{1/2} = 2.4$ d for whole body, $t_{1/2} = 2.3$ d for gonads, $t_{1/2} = 2.3$ d for gills, and $t_{1/2} = 2.2$ d for liver (Lemaire et al. 1990); elimination $t_{1/2} = 4.8 - 16$ d from mussel $M. edulis$; $t_{1/2} = 7$ d from polychaete $A. pacifica$, $t_{1/2} = 21.7$ d from Oyster; $t_{1/2} = 8.0$ d from clam $M. mercenaria$, $t_{1/2} = 8$ d from clam $R. cuneata$ (quoted, Meador et al. 1995); $t_{1/2} = 15 - 17$d for blue mussel $M. edulis$ 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

\[ \ln x = A + B/(T/K) + C \cdot \ln (T/K) \] (1)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Aqueous solubility (g/m³)</th>
<th>Henry’s law constant (Pa m³/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.00056</td>
<td>0.00061</td>
</tr>
<tr>
<td>15</td>
<td>0.00080</td>
<td>0.00082</td>
</tr>
<tr>
<td>20</td>
<td>0.00114</td>
<td>0.00113</td>
</tr>
<tr>
<td>25</td>
<td>0.00162</td>
<td>0.00158</td>
</tr>
<tr>
<td>30</td>
<td>0.00229</td>
<td>0.00224</td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{sol}}/(kJ \cdot mol^{-1}) = 50.6 \] at 25°C

\[ \ln K_{\text{AW}} = \Delta H/RT + \Delta S/R \]

\[ R = 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1} \]

\[ \Delta S/R = 11.90 \]

\[ \Delta H/R = 4690.88 \]

enthalpy of volatilization:

\[ \Delta H/(kJ \cdot mol^{-1}) = 39 \pm 3 \]

entropy of volatilization, \( \Delta S : \)

\[ T \Delta S/(kJ \cdot mol^{-1}) = 29 \pm 3 \] at 20°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: C₂₀H₁₂
Molecular Weight: 252.309
Melting Point (°C):
  181.4  (Lide 2003)
Boiling Point (°C):
  311  (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
  222.8  (Ruelle & Kesselring 1997; Passivirta et al. 1999)
  262.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔHₘₙ (kJ/mol):
  16.57  (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔSₘₙ (J/mol K):
  42.30  (differential scanning calorimetry, Hinckley et al. 1990)
  36.5  (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔSₘₙ = 56 J/mol K), F:
  0.0292  (mp at 181.4°C)
  0.010  (calculated, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°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  (27°C, 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*  (23°C, shake flask-fluorescence, measured range 8.6–31.7°C, Schwarz 1977)
  0.00732, 0.004; 0.0063 (quoted values; lit. mean, Pearlman et al. 1984)
log S₅ (mol/L) = –1.398 – 866.8/(T/K) (supercooled liquid, Passivirta et al. 1999)
ln x = –11.8754 – 2916.84/(T/K); temp range 5–50°C (regression eq. of literature data, Shiu & Ma 2000)
Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
  7.40 × 10⁻⁷  (Knudsen effusion method, extrapolated, Murray et al. 1974)
log (P/mmHg) = 9.736 – 6220/(T/K); temp range 359–423 K (Knudsen effusion method, Murray et al. 1974)
  7.58 × 10⁻²  (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (Pₚ/kPa) = 11.7417 – 6220/(T/K); temp range 358–423 K (Antoine eq., Stephenson & Malanowski 1987)
  3.20 × 10⁻³, 1.28 × 10⁻⁵ (20°C, literature solid Pₛ, converted to supercooled liquid Pₗ with ΔSₘₙ Bidleman & Foreman 1987)
  8.59 × 10⁻⁵ (PₛC, GC-RT correlation with pDₚ = –DDT as reference standard, Hinckley et al. 1990)
  2.53 × 10⁻³, 1.02 × 10⁻⁵ (supercooled liquid values Pₛ, converted from literature Pₛ with different ΔSₘₙ values, Hinckley et al. 1990)
log (Pₓ/Pₚ) = 11.11 – 4803/(T/K) (GC-RT correlation, Hinckley et al. 1990)
  1.29 × 10⁻⁴ (supercooled liquid values Pₚ, calculated from Yamasaki et al. 1984, Finizio et al. 1997)
  1.78 × 10⁻⁵, 1.78 × 10⁻⁶ (quoted supercooled liquid Pₛ from Hinckley et al. 1990; converted to solid Pₛ with fugacity ratio F, Passivirta et al. 1999)
log (Pₓ/Pₚ) = 12.15 – 5333/(T/K) (solid, Passivirta et al. 1999)
log (P_L/P_a) = 10.14 – 4467/(T/K) (supercooled liquid, Passivirta et al. 1999)

Henry’s Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations):
0.02 (calculated-P/C, Mackay et al. 1992)
log [H/(Pa m^3/mol)] = 11.64 – 3660/(T/K) (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW}:
6.44 (calculated-MCI $\chi$ as per Rekker & De Kort 1979, Ruepert et al. 1985)
7.40 (calculated-K_{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 K_{OA}:
11.13 (calculated, Finizio et al. 1997)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:
7.20 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
4.00 (predicted dissolved log K_{OC}, Broman et al. 1991)
6.11–7.90; 7.20–8.30 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.84; 6.12, 6.11, 6.62 20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants or Half-Lives:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:
k_1 = 0.13–0.36 mg g^{-1} h^{-1}; k_2 = 0.0031 h^{-1} (freshwater oligochaete from sedment, Van Hoof et al. 2001)

Half-Lives in the Environment:
Air: half-lives under simulated atmospheric conditions: t_{1/2} = 21.10 h in simulated sunlight, t_{1/2} = 5.38 h in simulated sunlight + ozone (0.2 ppm), t_{1/2} = 7.6 h in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983).
Surface water:
Groundwater:
Sediment:
Soil:
Biota: elimination t_{1/2} = 6.9–14.4 d from mussel *Mytilus edulis*; t_{1/2} = 30.1 d from Oyster, t_{1/2} = 4.7 d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

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**TABLE 4.1.1.44.1**
Reported aqueous solubilities of benzo[e]pyrene at various temperatures

<table>
<thead>
<tr>
<th>Schwarz 1977</th>
<th>shake flask-fluorescence</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/°C$</td>
<td>$S/g·m^{-3}$</td>
</tr>
<tr>
<td>8.6</td>
<td>$3.25 \times 10^{-3}$</td>
</tr>
<tr>
<td>14.0</td>
<td>$3.58 \times 10^{-3}$</td>
</tr>
<tr>
<td>17.0</td>
<td>$4.44 \times 10^{-3}$</td>
</tr>
<tr>
<td>17.5</td>
<td>$3.94 \times 10^{-3}$</td>
</tr>
<tr>
<td>t/°C</td>
<td>S/g·m⁻³</td>
</tr>
<tr>
<td>------</td>
<td>---------</td>
</tr>
<tr>
<td>20.2</td>
<td>4.79 × 10⁻³</td>
</tr>
<tr>
<td>23.2</td>
<td>5.35 × 10⁻³</td>
</tr>
<tr>
<td>23.0</td>
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<tr>
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<tr>
<td>29.2</td>
<td>6.48 × 10⁻³</td>
</tr>
<tr>
<td>31.7</td>
<td>6.81 × 10⁻³</td>
</tr>
</tbody>
</table>

\[ \Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 25.56 \]

at 25°C
4.1.1.45 Perylene

Common Name: Perylene
Synonym: peri-dinaphthalene
Chemical Name: perylene
CAS Registry No: 198-55-0
Molecular Formula: C$_{20}$H$_{12}$
Molecular Weight: 252.309
Melting Point (°C):
  277.76 (Lide 2003)
Boiling Point (°C):
  503 (Pearlman et al. 1984)
Density (g/cm$^3$ at 25°C):
  1.35 (Lide 2003)
Molar Volume (cm$^3$/mol):
  186.9 (25°C, calculated-density)
  222.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
  262.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
  23.51 (quoted, Tsonopoulos & Prausnitz 1971)
  31.753 (Ruelle & Kesselring 1997)
  31.88 (exptl., Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol 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°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
  0.00331 (mp at 277.76°C)
  0.00268 (calculated, Passivirta et al. 1999)
Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated and reported temperature dependence equations):
  0.0005 (27°C, shake flask-nephelometry Davis et al. 1942)
  < 0.0005 (Weimer & Prausnitz 1965)
  0.00011 (20°C, 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 $[S_L/(\text{mol/L})] = -0.306 - 1662/(T/K)$ (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
  log $[P/(\text{mmHg})] = 13.95 – 7260/(T/K)$; temp range 110–180°C (Knudsen effusion method, Hoyer & Peperle 1958)
  $5.31 \times 10^{-9}$ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
  log $[P/(\text{kPa})] = 13.075 – 7260/(T/K)$; temp range 383–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)
  log $[P/(\text{kPa})] = 12.9379 – 7210/(T/K)$; temp range 383–516 K (Antoine eq.-II, Stephenson & Malanowski 1987)
  $7.00 \times 10^{-7}$ (quoted, Riederer 1990)
  $1.84 \times 10^{-8*}$ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 118–210°C, Oja & Suuberg 1998)
  $\ln [(P/(\text{Pa})] = 35.702 – 15955/(T/K)$; temp range 391–424 K (Clausius-Clapeyron eq., Knudsen effusion, Oja & Suuberg 1998)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

1.40 × 10⁻⁸; 5.22 × 10⁻⁶ (quoted solid Pₛ from Mackay et al. 1992; converted to supercooled liquid Pₐ with fugacity ratio F, Passivirta et al. 1999)

\[
\log (Pₛ/Pₐ) = 12.53 - 6074/(T/K) \quad (\text{solid, Passivirta et al. 1999})
\]

\[
\log (Pₛ/Pₐ) = 9.53 - 4414/(T/K) \quad (\text{supercooled liquid, Passivirta et al. 1999})
\]

4.88 × 10⁻⁶ (supercooled liquid Pₛ, calibrated GC-RT correlation, Lei et al. 2002)

\[
\log (Pₛ/Pₐ) = -4694/(T/K) + 10.43; \quad \Delta H_{\text{vap.}} = -89.9 \text{kJ·mol}⁻¹ \quad (\text{GC-RT correlation, Lei et al. 2002})
\]

Henry’s Law Constant (Pa m³/mol at 25°C and the report temperature dependence equations):

0.440 \quad (\text{calculated-P/C, Riederer 1990})

\[
\log \left[ \frac{H}{(\text{Pa m}³/\text{mol})} \right] = 9.84 - 2752/(T/K), \quad (\text{Passivirta et al. 1999})
\]

Octanol/Water Partition Coefficient, log K_{OW}:

6.30, 5.10 \quad (\text{HPLC-RV predicted, Brooke et al. 1986})

5.30 \quad (\text{HPLC-RV measured, Brooke et al. 1986})

5.82 \quad (\text{HPLC-RT correlation, Wang et al. 1986})

6.25 \quad (\text{recommended, Sangster 1989, 1994})

6.40 \quad (\text{Bayona et al. 1991})

5.82 \quad (\text{recommended, Hansch et al. 1995})

6.50 \quad (\text{shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schräder 1999})

6.25; 6.53 \quad (\text{quoted lit.; calculated, Passivirta et al. 1999})

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

3.86, 3.73 \quad (Daphnia pulex, kinetic estimation, Southworth et al. 1978)

4.36 \quad (\text{activated sludge, Freitag et al. 1984})

3.30, 4.36, < 1.0 \quad (\text{algae, activated sludge, fish, Klein et al. 1984})

3.85 \quad (Daphnia pulex, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)

3.30, 4.36, < 1.0 \quad (\text{algae, activated sludge, fish, Freitag et al. 1985})

3.86 \quad (Daphnia magna, Newsted & Giesy 1987)

1.196, –0.398 \quad (Polychaete sp, Capitella capitata, Bayona et al. 1991)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

6.39–7.93 \quad (\text{range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001})

5.88; 6.73, 6.63, 6.76 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3-solvophobic approach, Krauss & Wilcke 2001)

6.30; 5.89; 4.15–6.38 (calculated-K_{OW}; calculated-solubility; quoted lit. range, Schlautman & Morgan 1993a)

6.05 at pH 4, 5.98 at pH 7, 5.71 at pH 10 in 0.001 M NaCl; 6.01 at pH 4, 5.95 at pH 7, 5.29 at pH 10 in 0.01 M NaCl; 5.98 at pH 4, 5.67 at pH 7, 4.86 at pH 10 in 0.1 M NaCl; 5.97 at pH 4, 5.61 at pH 7, 4.78 at pH 10 in 1 mM Ca²⁺ in 0.1M total ionic strength solutions (shake flask/fluorescence, dissolved humic substances-humic acid; Schlautman & Morgan 1993)

5.17 at pH 4 in 0.001 M NaCl; 5.14 at pH 4 in 0.01 M NaCl; 5.08 at pH 4 in 0.1 M NaCl; 5.11 at pH 4 in 1 mM Ca²⁺ in 0.1 M total ionic strength solutions (shake flask/fluorescence, dissolved humic substances-fulvic acid; Schlautman & Morgan 1993b)

5.82 at pH 4, < 4.49 at pH 7, < 4.18 at pH 10 in 0.001 M NaCl; 5.65 at pH 4, < 4.46 at pH 7, < 3.85 at pH 10 in 0.01 M NaCl; 5.67 at pH 4, < 4.17 at pH 7, < 3.78 at pH 10 in 0.1 M NaCl; 5.74 at pH 4, 5.02 at pH 7, 4.43 at pH 10 in 1 mM Ca²⁺ in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-humic acid; Schlautman & Morgan 1993b)

< 3.48 at pH 4 in 0.001 M NaCl; < 3.30 at pH 4 in 0.01 M NaCl; < 3.48 at pH 4 in 0.1 M NaCl; < 3.48 at pH 4 in 1 mM Ca²⁺ in 0.1 M total ionic strength solutions (shake flask/fluorescence, adsorbed humic substances-fulvic acid; Schlautman & Morgan 1993b)

6.00 \quad (\text{soil humic acid, shake flask-HPLC/UV, Cho et al. 2002})
Environmental Fate Rate Constants, \( k \) or Half-Lives, \( t_{1/2} \):

- **Volatilization**: sublimation \( k < 1 \times 10^{-5} \, \text{s}^{-1} \) from glass surface was measured at 24°C at an airflow rate of 3 L/min (Cope & Kalkwarf 1987).

- **Photolysis**:
  - half-lives on different atmospheric particulate substrates (appr. 25 \( \mu \text{g/g} \) on substrate): \( t_{1/2} = 3.9 \, \text{h} \) on silica gel, \( t_{1/2} = 1.2 \, \text{h} \) on alumina and \( t_{1/2} = 35 \, \text{h} \) on fly ash (Behymer & Hites 1985)
  - ozonation \( k < 4.7 \times 10^{-5} \, \text{m/s} \) was measured from glass surface at 24°C with \([\text{O}_3]\) = 0.16 ppm and light intensity of 1.3 kW/m² (Cope & Kalkwarf 1987)
  - photodegradation \( k = 0.0152 \, \text{min}^{-1} \) and \( t_{1/2} = 0.78 \, \text{h} \) in ethanol-water (2:3, v/v) solution for initial concentration of 5.0 ppm by high pressure mercury lamp or sunlight (Wang et al. 1991)
  - photodegradation \( k = 4.4 \times 10^{-4} \, \text{s}^{-1} \) in surface water during the summertime at mid-latitude (Fasnacht & Blough 2002)

- **Hydrolysis**:

- **Oxidation**:

- **Biodegradation**:

- **Biotransformation**:

- **Bioconcentration, Uptake (\( k_1 \)) and Elimination (\( k_2 \)) Rate Constants**:
  - \( k_1 = 752 \, \text{h}^{-1} \); \( k_2 = 0.139 \, \text{h}^{-1} \) (\textit{Daphnia pulex}, Southworth et al. 1978)
  - \( \log k_1 = 2.88 \, \text{h}^{-1} \); \( \log k_2 = -0.86 \, \text{h}^{-1} \) (\textit{Daphnia pulex}, correlated as per Mackay & Hughes 1984, Hawker & Connell 1986)
  - \( k_1 = 0.12-0.38 \, \text{mg g}^{-1} \, \text{h}^{-1} \); \( k_2 = 0.0034 \, \text{h}^{-1} \) (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

- **Air**: direct photolysis \( t_{1/2} = 0.53 \, \text{h} \) (predicted- QSPR) in atmospheric aerosol (Chen et al. 2001).
- **Surface water**: photolysis \( t_{1/2} = 0.78 \, \text{h} \) (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: \( t_{1/2} = 2.0 \, \text{d} \) from rainbow trout, \( t_{1/2} = 26.2 \, \text{d} \) from clam \textit{Mya arenaria}, \( t_{1/2} = 6.3-13.3 \, \text{d} \) from mussel \textit{Mytilus edulis}; \( t_{1/2} = 9.2 \, \text{d} \) from Oyster, \( t_{1/2} = 1.2 \, \text{d} \) from shrimp, \( t_{1/2} = 5.7 \, \text{d} \) from polychaete \textit{Nereis virens}, \( t_{1/2} = 8.0 \, \text{d} \) from clam \textit{Mercenario mercenaria} (quoted, Meador et al. 1995).

### TABLE 4.1.1.45.1

<table>
<thead>
<tr>
<th>Reported vapor pressures of perylene at various temperatures and the coefficients for the vapor pressure equations</th>
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<tr>
<td>( \log P = A - B/(T/K) )</td>
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<tr>
<td>( \log P = A - B/(C + t/°C) )</td>
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<th>( Hoyer &amp; Peperle 1958 )</th>
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<tr>
<td>( \text{effusion} )</td>
<td>( \text{Knudsen effusion} )</td>
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<td>data presented by equation</td>
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<tr>
<td>eq. 1</td>
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TABLE 4.1.1.45.1 (Continued)

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<th>Oja &amp; Suuberg 1998</th>
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<td>for temp range 391–424 K</td>
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<td>∆H_{sub}/(kJ/mol)</td>
<td>= 132.6</td>
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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: C\textsubscript{20}H\textsubscript{16}
Molecular Weight: 256.341
Melting Point (°C): 122.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm\textsuperscript{3} at 20°C):
Molar Volume (cm\textsuperscript{3}/mol): 245.8 (Ruelle & Kesselring 1997)
292.7 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol): 104.56 (Kelley & Rice 1964)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol): 22.09 (Kelley & Rice 1964)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.111 (mp at 122.5°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated):
0.043 (27°C, shake flask-nephelometry, Davis et al. 1942)
0.061 (shake flask-fluorescence, Mackay & Shiu 1977)
0.053 (24°C, shake flask-nephelometry, Hollifield 1979)
0.025 (24°C, 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°C and reported temperature dependence equations):
3.73 × 10\textsuperscript{-7} (solid vapor pressure, extrapolated, effusion method, Kelley & Rice 1974)
3.70 × 10\textsuperscript{-6} (extrapolated, supercooled liquid value $P_L$, Kelley & Rice 1974)
$\log (P_v/mmHg) = 15.108 – 7051/(T/K)$; temp range: 106–122°C (effusion method, Kelley & Rice 1964)
$\log (P_v/mmHg) = 12.232 – 5987/(T/K)$; temp range: 122–135°C (effusion method, Kelley & Rice 1964)
3.84 × 10\textsuperscript{-7} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_v/kPa) = 14.233 – 7051/(T/K)$; temp range 379–396 K (Antoine eq.-I, Stephenson & Malanowski 1987)
$\log (P_v/kPa) = 10.70417 – 5629.911/(T/K)$; temp range 379–390 K (Antoine eq.-II, Stephenson & Malanowski 1987)
$\log (P_v/kPa) = -4643/(T/K) + 10.38$; $\Delta H_{vap.} = -88.9$ kJ·mol\textsuperscript{-1} (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m\textsuperscript{3}/mol):
Octanol/Water Partition Coefficient, log $K_{ow}$:
5.98 (shake flask-LSC, concn. ratio, Means et al. 1979)
5.80 (shake flask-LSC, Means et al. 1980b)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log $BCF$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:

Volatile:

Hydrolysis:

Photolysis:

Oxidation:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.32–3.2$ h, based on estimated photodegradation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 480–672$ h, based on aerobic soil die-away test data (Howard et al. 1991).

Groundwater: $t_{1/2} = 960–1344$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation rate constant $k = 0.0339 \text{ d}^{-1}$ with $t_{1/2} = 20$ d for Kidman sandy loam soil and $k = 0.0252 \text{ d}^{-1}$ with $t_{1/2} = 28$ d for McLaurin sandy loam soil (Park et al. 1990); $t_{1/2} \approx 480–672$ 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: C_{20}H_{16}
Molecular Weight: 256.341
Melting Point (°C):
122  (Yalkowsky et al. 1983; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³ at 20°C):
245.8  (Ruelle & Kesselring 1997)
292.7  (calculated-Le Bas method at normal boiling point)
Entrophy of Fusion, ΔS_{fus} (J/mol K):
54.81  (Kelley & Rice 1974)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.112 (mp at 122°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
0.0435  (27°C, shake flask-nephelometry, Davis et al. 1942)
0.0435  (recommended, Shaw 1989)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
log (P/mmHg) = 15.108 – 7051/(T/K); temp range: 106–135°C (effusion method, Kelley & Rice 1964)
log (P/mmHg) = 12.232 – 5897/(T/K) (liquid, effusion method, Kelley & Rice 1964)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
6.93  (calculated-fragment const., Yalkowsky et al. 1983)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k or Half-Lives, t_½:
Half-Lives in the Environment:
4.1.1.48  3-Methylcholanthrene

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: C_{21}H_{16}
Molecular Weight: 268.352
Melting Point (°C):
180  (Bjørseth 1983)
Boiling Point (°C):
Density (g/cm³ at 20°C):
1.28  (Lide 2003)
Molar Volume (cm³/mol):
247.8  (Ruelle & Kesselring 1997)
209.6  (20°C, calculated-density)
296.0  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0301 (mp at 180°C)
0.003  (Mackay et al. 1980)
Water Solubility (g/m³ or mg/L at 25°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°C and reported temperature dependence equations):
log (P/µmHg) = 13.168 – 6643/(T/K); temp range 128–152°C (effusion method, Kelley & Rice 1964)
1.03 × 10⁻⁷ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P_0/µPa) = 12.293 – 6643/(T/K); temp range 401–425 K (Antoine eq., Stephenson & Malanowski 1987)
1.48 × 10⁻⁶ (supercooled liquid P_f, calibrated GC-RT correlation, Lei et al. 2002)
log (P_f/µPa) = –4901/(T/K) + 10.61; ΔH_{vap.} = –93.8 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{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 ± 0.50  (recommended, Sangster 1989)
6.45  (recommended, Sangster 1993)
6.42  (recommended, Hansch et al. 1995)
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:
- 4.12 ($Daphnia magna$, McCarthy et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:
- 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 $K_p$ versus substrate properties, calculated-KOW, Means et al. 1980)
- 4.02 (soil, calculated-KOW, Briggs 1981)
- 6.18 (soil, calculated-KOW, Means et al. 1982)
- 5.07 (soil, calculated-KOW, Chiou et al. 1983)

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_\text{½}$:

Volatilization:

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: photooxidation $t_\text{½} = 0.317–3.17$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aerobic $t_\text{½} = 14616–33600$ h, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991);

anaerobic $t_\text{½} = 58464–134400$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake ($k_1$) and Elimination ($k_2$) Rate Constants:

Half-Lives in the Environment:

Air: $t_\text{½} = 0.317–3.17$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_\text{½} = 14616–33600$ h, based on mineralization half-life in fresh water and estuarine ecosystems (Heitkamp 1988; quoted, Howard et al. 1991).

Groundwater: $t_\text{½} = 29232–672000$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_\text{½} = 14616–33600$ 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: C_{22}H_{12}
Molecular Weight: 276.330
Melting Point (°C):
272.5 (Lide 2003)
Boiling Point (°C):
525 (Pearlman et al. 1984)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
233.8 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
277.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
17.365 (Ruelle & Kesselring 1997)
17.37 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{ fus} (J/mol K):
31.34, 43.2 (exptl., calculated-group additivity method, Chickos et al. 1999)
31.4 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F = 0.00373 (mp at 272.5°C)
0.039 (calculated, ΔS_{ fus} = 31.4 J/mol K, Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°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 [S_L/(mol/L)] = – 2.073 – 908.7/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations):
1.39 × 10⁻⁸ (Knudsen effusion method, Murray et al. 1974)
log (P/atom) = 9.519 – 6674/(T/K); temp range: 389–468 K (Knudsen effusion method, Murray et al. 1974)
1.33 × 10⁻⁸ (20°C, estimated, Callahan et al. 1979)
6.69 × 10⁻⁷ (Yamasaki et al. 1984)
1.38 × 10⁻⁸; 7.51 × 10⁻⁹ (extrapolated-Antoine eq. I, II, Stephenson & Malanowski 1987)
log (Pₚ/kPa) = 11.5247 – 6674/(T/K); temp range 389–468 K (Antoine eq.-I, Stephenson & Malanowski 1987)
log (Pₚ/kPa) = 10.945 – 6580/(T/K); temp range 391–513 K (Antoine eq.-II, Stephenson & Malanowski 1987)
7.20 × 10⁻⁶; 1.84 × 10⁻⁶ (quoted solid Pₚ from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)
log (P_L/Pa) = 12.40 – 5824/(T/K) (solid, Passivirta et al. 1999)
log (P_L/Pa) = 10.76 – 4915/(T/K) (supercooled liquid, Passivirta et al. 1999)
4.28 × 10⁻⁷ (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)
log (P_L/Pa) = –5018/(T/K) + 10.46; ΔH_{ vap} = –96.1 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m^3/mol at 25°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* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992) 
\[
\log (H/(Pa \cdot m^3/mol)) = 12.83 - 4006/(T/K) 
\] (Passivirta et al. 1999)

0.0278(20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001) 
\[
\log K_{AW} = -0.651 - 1258/(T/K) 
\] (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{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/fluor., De Maagd et al. 1998)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

5.54 (microorganisms-water, calculated from K_{OW}, Mabey et al. 1982)
4.45 (Daphnia magna, Newsted & Giesy 1987)

Sorption Partition Coefficient, log K_{OC} at 25°C or as indicated:

6.70 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
7.215 (10°C), 7.08, 6.93 (20°C), 6.68 (35°C), 6.46, 6.51 (45°C) (log K_{DOC} - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.80 (20°C, log K_{POC} - particulate organic material from lake, Lüers & ten Hulscher 1996)
6.82–8.25; 6.20–6.20 (range, calculated from sequential desorption of 11 urban soils; lit. range, Krauss & Wilcke 2001)
5.87; 6.84, 6.82, 7.26 (20°C, batch equilibrium, A2 alluvial grassland soil; calculated values of expt 1,2,3- solvophob approach, Krauss & Wilcke 2001)

Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:

Volutilization:
Photolysis: half-lives on different atmospheric particulate substrates (approx. 25 μg/g on substrate): t_{1/2} = 7.0 h on silica gel, t_{1/2} = 22 h on alumina and t_{1/2} = 29 h on fly ash (Behymer & Hites 1985); first order daytime photodegradation rate constants for adsorption on wood soot particles in an outdoor Teflon chamber: k = 0.0077 min^{-1} with 1000–2000 ng/mg loading and k = 0.0116 min^{-1} with 30–350 ng/mg loading (Kamens et al. 1988);
direct photolysis t_{1/2}(obs) = 0.89 h, t_{1/2}(calc) = 0.86 h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Oxidation: rate constants k < 60 M^{-1} h^{-1} for singlet oxygen and k < 6 M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982); photooxidation t_{1/2} = 0.321–3.21 h, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aerobic t_{1/2} = 14160–15600 h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; quoted, Howard et al. 1991); anaerobic t_{1/2} = 56640–62400 h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; quoted, Howard et al. 1991).

Biotransformation: estimated to be 3 × 10^{-12} mL cell^{-1} h^{-1} for bacteria (Mabey et al. 1982).

Bioconcentration, Uptake (k_{1}) and Elimination (k_{2}) Rate Constants:

k_{1} = 0.076–0.21 mg g^{-1} h^{-1}; k_{2} = 0.0012–0.0014 h^{-1} (freshwater oligochaete from sediment, Van Hoof et al. 2001)
Half-Lives in the Environment:

Air: $t_{1/2} = 0.321–3.21$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991); $t_{1/2} = 0.6$ h for adsorption on wood soot particles in an outdoor Teflon chamber with an estimated first order rate constant $k = 0.0179$ min$^{-1}$ at 1 cal cm$^{-2}$ min$^{-1}$, 10 g/m$^3$ H$_2$O and 20°C (Kamens et al. 1988).

Surface water: $t_{1/2} = 14160–15600$ h, based on aerobic soil die-away test data at 10–30°C (Coover & Sims 1987; quoted, Howard et al. 1991).


Sediment:

Soil: $t_{1/2} = 14160–15600$ h, based on aerobic soil die-away test data (Coover & Sims 1987; quoted, Howard et al. 1991);

$t_{1/2} > 50$ d (Ryan et al. 1988);

mean $t_{1/2} = 9.1$ yr for Luddington soil (Wild et al. 1991).

Biota: elimination $t_{1/2} = 12.4$ d from Oyster, $t_{1/2} = 4.8$ d from clam *Mercenaria mercenaria* (quoted, Meador et al. 1995).

### TABLE 4.1.1.49.1

<table>
<thead>
<tr>
<th>ten Hulscher et al. 1992</th>
<th>Reported Henry’s law constants of benzo[ghi]perylene at various temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t/°C</strong></td>
<td><strong>H/(Pa m$^3$/mol)</strong></td>
</tr>
<tr>
<td>10.0</td>
<td>0.019</td>
</tr>
<tr>
<td>20.0</td>
<td>0.027</td>
</tr>
<tr>
<td>35.0</td>
<td>0.052</td>
</tr>
<tr>
<td>40.1</td>
<td>0.054</td>
</tr>
<tr>
<td>45.0</td>
<td>0.066</td>
</tr>
<tr>
<td>55.0</td>
<td>0.087</td>
</tr>
</tbody>
</table>

enthalpy of volatilization:

$\Delta H_{vol}/(kJ\cdot mol^{-1}) = 26.1\pm1.0$

entropy of volatilization, $\Delta S$

$T\Delta S_{vol}/(kJ\cdot mol^{-1}) = 15.9\pm1.3$

at 20°C

$\ln K_{AW} = -\Delta H_{vol}/RT + \Delta S_{vol}/R$

$R = 8.314$ Pa m$^3$ mol$^{-1}$ K$^{-1}$
4.1.1.50 Indeno[1,2,3-cd]pyrene

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: C_{22}H_{12}
Molecular Weight: 276.330
Melting Point (°C):
162 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
233.8 (Ruelle & Kesselring 1997, Passivirta et al. 1999)
283.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
21.51 (Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
49.41, 36.0 (exptl., calculated-group additivity method, Chickos et al. 1999)
56.5 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0453 (mp at 162°C)
0.043 (Passivirta et al. 1999)
Water Solubility (g/m³ or mg/L at 25°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 [S_L/(mol/L)] = −0.758 − 1631/(T/K) (supercooled liquid, Passivirta et al. 1999)
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
1.33 × 10⁻⁷ (estimated, Callahan et al. 1979)
1.00 × 10⁻⁴; 2.32 × 10⁻⁷ (quoted solid P_s from Mackay et al. 1992; converted to supercooled liquid P_L with fugacity ratio F, Passivirta et al. 1999)
log (P_s/P_a) = 12.56 − 6126/(T/K) (solid, Passivirta et al. 1999)
log (P_L/P_a) = 9.60 − 4839/(T/K) (supercooled liquid, Passivirta et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
0.029* (20°C, gas stripping-HPLC/fluorescence, measured range 10–55°C, ten Hulscher et al. 1992)
log [H/(Pa·m³/mol)] = 10.36 − 3208/(T/K) (Passivirta et al. 1999)
0.0285 (20°C, selected from reported experimentally measured values, Staudinger & Roberts 1996, 2001)
log K_{AW} = 0.033 − 1455/(T/K) (van’t Hoff eq. derived from literature data, Staudinger & Roberts 2001)
Octanol/Water Partition Coefficient, log K_{OW}:
7.66 (calculated-π substituent const., Callahan et al. 1979)
8.20 (calculated, Broman et al. 1991)
6.72 (calculated, Passivirta et al. 1999)
Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons

Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

8.00 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
6.93 (10°C), 6.88, 6.84 (20°C), 6.42 (35°C), 6.32, 6.31 (45°C) (log $K_{DOC}$ - dissolved organic material from lake, gas-purge technique-HPLC/fluorescence, Lüers & ten Hulscher 1996)
6.80 (20°C, log $K_{POC}$ - particulate organic material from lake, Lüers & ten Hulscher 1996)

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 0.067–0.20$ mg g$^{-1}$ h$^{-1}$; $k_2 = 0.0010–0.0013$ h$^{-1}$ (freshwater oligochaete from sediment, Van Hoof et al. 2001)

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>$t$/°C</th>
<th>$H/(Pa \cdot m^3/mol)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>0.018</td>
</tr>
<tr>
<td>20.0</td>
<td>0.029</td>
</tr>
<tr>
<td>35.0</td>
<td>0.057</td>
</tr>
<tr>
<td>40.1</td>
<td>0.061</td>
</tr>
<tr>
<td>45.0</td>
<td>0.077</td>
</tr>
<tr>
<td>55.0</td>
<td>0.105</td>
</tr>
</tbody>
</table>

Reported Henry’s law constants of indeno[123-cd]pyrene at various temperatures

ten Hulscher et al. 1992

gas stripping-HPLC/fluor.

enthalpy of volatilization: $\Delta H/(kJ\cdot mol^{-1}) = 30.0 \pm 1.1$

entropy of volatilization, $\Delta S$: $T\Delta S/(J\cdot K^{-1}\cdot mol^{-1}) = 19.9\pm1.3$

at 20°C

$\ln K_{AW} = -\Delta H/RT + \Delta S/R$

$R = 8.314$ Pa m$^3$ mol$^{-1}$ K$^{-1}$

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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: C_{22}H_{14}
Molecular Weight: 278.346
Melting Point (°C): 205 (Bjørseth 1983; Lide 2003)
Boiling Point (°C): 518 (Weast 1982–83)
Density (g/cm³ at 20°C): 299.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol): 25.82 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K): 46.65, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0171 (mp at 205°C)
Water Solubility (g/m³ or mg/L at 25°C): 0.0016 (generator column-HPLC/UV, Billington et al. 1988)
Vapor Pressure (Pa at 25°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 × 10^{-9} (effusion method, extrapolated, De Kruif 1980)
log (P/Pa) = 16.25 – 7322.2/(T/K); temp range: 152–179°C (torsion-effusion, de Kruif 1980)
log (P/Pa) = 16.011 – 7207.2/(T/K); temp range: 152–179°C (weighing-effusion, de Kruif 1980)
log (P/Pa) = 16.131 – 7265/(T/K); temp range: 152–179°C (mean, de Kruif 1980)
3.44 × 10^{-7} (supercooled liquid P_{L}, calibrated GC-RT correlation, Lei et al. 2002)
log (P_{L}/Pa) = –5094/(T/K) + 10.62; ΔH_{vap} = –97.5 kJ·mol^{-1} (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
7.19 (calculated, Miller et al. 1985)
7.11 (calculated-MCI χ 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 ± 0.19, 6.48 ± 0.78 (HPLC-k’ correlation: ODS column; Diol column, Helweg et al. 1997)
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, \( \log K_{OC} \):

6.54 \hspace{1cm} \text{(humic acid, HPLC-k' correlation, Nielsen et al. 1997)}

Environmental Fate Rate Constants, \( k \) or Half-Lives, \( t_{1/2} \):

Half-Lives in the Environment:

Air: half-lives under simulated atmospheric conditions: \( t_{1/2} = 9.20 \) h in simulated sunlight, \( t_{1/2} = 4.60 \) h in simulated sunlight + ozone (0.2 ppm), \( t_{1/2} = 3.82 \) h in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983).

\[ \text{TABLE 4.1.1.51.1} \]

Reported vapor pressures of dibenz[a,c]anthracene at various temperatures and the coefficients for the vapor pressure equations

\[
\begin{align*}
\log P &= A - B/(T/K) \quad (1) \\
\ln P &= A - B/(T/K) \quad (1a) \\
\log P &= A - B/(C + t/°C) \quad (2) \\
\ln P &= A - B/(C + t/°C) \quad (2a) \\
\log P &= A - B/(C + T/K) \quad (3) \\
\log P &= A - B/(T/K) - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

de Kruif 1980

torsion-, weighing effusion

\[
\begin{array}{c|c}
t/°C & P/Pa \\
\hline
151.65 & 0.1 \\
158.52 & 0.2 \\
163.08 & 0.3 \\
166.38 & 0.4 \\
168.97 & 0.5 \\
171.11 & 0.6 \\
172.94 & 0.7 \\
174.53 & 0.8 \\
175.95 & 0.9 \\
177.22 & 1.0 \\
298.15 & 1.3 \times 10^{-9} \\
\hline
\end{array}
\]

Extrapolated

\( \Delta H_{sub}/(kJ \text{ mol}^{-1}) = 138.0 \)

\[ \text{FIGURE 4.1.1.51.1} \] 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: C$_{22}$H$_{14}$
Molecular Weight: 278.346
Melting Point (°C): 269.5 (Lide 2003)
Boiling Point (°C): 524 (Weast 1977)
Density (g/cm$^3$ at 20°C): 
Molar Volume (cm$^3$/mol):
- 252.6 (Ruelle & Kesselring 1997; Passivirta et al. 1999)
- 299.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
- 31.165 (Ruelle & Kesselring 1997)
- 31.16 (exptl., Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
- 58.26, 44.0 (exptl., calculated-group additivity method, Chickos et al. 1999)
- 57.3 (Passivirta et al. 1999)
Fugacity Ratio at 25°C (assuming $\Delta S_{fus}$ = 56 J/mol K), F: 0.00389 (mp at 269.5°C)
- 0.00389 (calculated, Passivirta et al. 1999)

Water Solubility (g/m$^3$ or mg/L at 25°C or as indicated and the reported temperature dependence equations):
- 0.0005 (27°C, 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 $[S_L/(mol/L)] = -1.409 - 1631/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
- $1.33 \times 10^{-8}$ (20°C, estimated, Callahan et al. 1979)
- $3.70 \times 10^{-10}$ (effusion method, De Kruif 1980)
log (P/Pa) = 16.049 – 7395.4/(T/K); temp range: 163–189°C (torsion-effusion, de Kruif 1980)
log (P/Pa) = 15.876 – 7312/(T/K); temp range: 163–189°C (weighing-effusion, de Kruif 1980)
log (P/Pa) = 15.962 – 7730/(T/K); temp range: 163–189°C (mean, de Kruif 1980)
4.25 $\times 10^{-10}$ (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
log (P$_s$/kPa) = 12.515 – 7420/(T/K); temp range 403–513 K (Antoine eq., Stephenson & Malanowski 1987)
3.70 $\times 10^{-10}$; 9.31 $\times 10^{-8}$ (quoted solid P$_s$ from Mackay et al. 1992; converted to supercooled liquid P$_L$ with fugacity ratio F, Passivirta et al. 1999)
log (P$_s$/Pa) = 12.82 – 5824/(T/K) (solid, Passivirta et al. 1999)
log (P$_s$/Pa) = 9.82 – 5002/(T/K) (supercooled liquid, Passivirta et al. 1999)
2.51 $\times 10^{-7}$ (supercooled liquid P$_L$, calibrated GC-RT correlation, Lei et al. 2002)
log (P$_L$/Pa) = –5193/(T/K) + 10.82; $\Delta H_{vap.} = –99.4$ kJ·mol$^{-1}$ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m^3/mol at 25°C and reported temperature dependence equations):

- 0.0074 (calculated-P/C, Mabey et al. 1982)
- 0.0076 (calculated-P/C, Eastcott et al. 1988)
- \( \log \left[ \frac{H}{(\text{Pa m}^3/\text{mol})} \right] = 11.23 – \frac{3371}{(T/\text{K})} \), (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, \( \log K_{\text{ow}} \):

- 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 ± 0.40 (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 ± 0.19, 6.60 ± 0.78 (HPLC-k′ correlation: ODS column; Diol column, Helweg et al. 1997)

Octanol/Air Partition Coefficient, \( \log K_{\text{oa}} \):

Bioconcentration Factor, \( \log BCF \):

- 5.84 (microorganisms-water, calculated from \( K_{\text{ow}} \), Mabey et al. 1982)
- 4.63 (activated sludge, Freitag et al. 1984)
- 3.38, 4.63, 1.0 (algae, activated sludge, fish, Freitag et al. 1985)
- 4.00 (Daphnia magna, Newsted & Giesy 1987)

Sorption Partition Coefficient, \( \log K_{\text{oc}} \):

- 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 \( k_p \) versus substrate properties, calculated-\( K_{\text{ow}} \), Means et al. 1980b)
- 6.22; 6.11, 5.30, 5.62 (quoted; calculated-\( K_{\text{ow}} \), calculated-S and mp, calculated-S, Karickhoff 1981)
- 6.52 (calculated-\( K_{\text{ow}} \), Mabey et al. 1982)
- 5.20 (calculated, Pavlou 1987)
- 6.31; 6.44; 3.75–5.77 (soil, quoted exptl.; calculated-MCI \( \chi \), calculated-\( K_{\text{ow}} \) range, Sabljic 1987a,b)
- 5.77 (soil, calculated-\( K_{\text{ow}} \) based on model of Karickhoff et al. 1979, Sabljic 1987b)
- 5.66 (soil, calculated-\( K_{\text{ow}} \) based on model of Means et al. 1982, Sabljic 1987b)
- 4.60 (soil, calculated-\( K_{\text{ow}} \) based on model of Chiou et al. 1983, Sabljic 1987b)
- 4.61 (soil, calculated-\( K_{\text{ow}} \) based on model of Kenaga 1980, Sabljic 1987b)
- 3.75 (soil, calculated-\( K_{\text{ow}} \) based on model of Briggs 1981, Sabljic 1987b)
- 6.22 (calculated-MCI \( \chi \), 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 (20°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, \( t_{1/2} \):

Volatilization:

Photolysis: atmospheric and aqueous photolysis \( t_{1/2} = 782 \) h, based on measured rate of photolysis in heptane under November sunlight (Muel & Saguem 1985; quoted, Howard et al. 1991) and \( t_{1/2} = 6 \) 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 \( k(\text{exptl}) = 0.014 \text{ min}^{-1} \) with the calculated \( t_{1/2} = 0.83 \) h and the predicted \( k = 0.0216 \text{ min}^{-1} \) calculated by QSPR method in aqueous solution when irradiated with a 500 W medium pressure mercury lamp (Chen et al. 1996); direct photolysis \( t_{1/2}(\text{obs.}) = 0.31 \) h, \( t_{1/2} = 0.38 \) h predicted by QSPR method in atmospheric aerosol (Chen et al. 2001).
Oxidation: rate constant \( k = 5 \times 10^8 \text{ M}^{-1} \text{ h}^{-1} \) for singlet oxygen and \( k = 1.5 \times 10^4 \text{ M}^{-1} \text{ h}^{-1} \) for peroxy radical (Mabey et al. 1982);
photooxidation \( t_{1/2} = 0.428-4.28 \text{ h} \), 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 \( t_{1/2} = 8664-22560 \text{ h} \), based on aerobic soil die-away test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);
\( k = 0.0019 \text{ d}^{-1} \) with \( t_{1/2} = 361 \text{ d} \) for Kidman sandy loam and \( k = 0.0017 \text{ d}^{-1} \) with \( t_{1/2} = 420 \text{ d} \) for McLarin sandy loam all at –0.33 bar soil moisture (Park et al. 1990).

Biotransformation: estimated to be \( 3 \times 10^{-12} \text{ mL cell}^{-1} \text{ h}^{-1} \) for bacteria (Mabey et al. 1982).

Biocencentration, Uptake \( (k_1) \) and Elimination \( (k_2) \) Rate Constants:

Half-Lives in the Environment:
Air: half-lives under simulated atmospheric conditions: \( t_{1/2} = 9.6 \text{ h} \) in simulated sunlight, \( t_{1/2} = 4.8 \text{ h} \) in simulated sunlight + ozone (0.2 ppm), \( t_{1/2} = 2.71 \text{ h} \) in dark reaction ozone (0.2 ppm) (Katz et al. 1979; quoted, Bjørseth & Olufsen 1983);
\( t_{1/2} = 0.428-4.28 \text{ h} \), based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: \( t_{1/2} = 6-782 \text{ h} \), based on sunlight photolysis half-life in water (Smith et al. 1978; Muel & Saguem 1985; quoted, Howard et al. 1991);
photolysis \( t_{1/2} = 0.83 \text{ h} \) in aqueous solution when irradiated with a 500 W medium-pressure mercury lamp (Chen et al. 1996).

Groundwater: \( t_{1/2} = 17328-45120 \text{ h} \), based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation rate constant \( k = 0.0019 \text{ d}^{-1} \) with \( t_{1/2} = 361 \text{ d} \) for Kidman sandy loam soil and \( k = 0.117 \text{ d}^{-1} \) with \( t_{1/2} = 420 \text{ d} \) for McLaurin sandy loam soil (Park et al. 1990);
\( t_{1/2} \approx 8664-22560 \text{ h} \), based on aerobic soil dieaway test data (Coover & Sims 1987; Sims 1990; quoted, Howard et al. 1991);
mean \( t_{1/2} = 20.607 \text{ wk} \) (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

<table>
<thead>
<tr>
<th>( T/\text{°C} )</th>
<th>( P/\text{Pa} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>160.38</td>
<td>0.1</td>
</tr>
<tr>
<td>168.21</td>
<td>0.2</td>
</tr>
<tr>
<td>172.93</td>
<td>0.3</td>
</tr>
<tr>
<td>176.33</td>
<td>0.4</td>
</tr>
<tr>
<td>179.01</td>
<td>0.5</td>
</tr>
<tr>
<td>181.22</td>
<td>0.6</td>
</tr>
<tr>
<td>183.11</td>
<td>0.7</td>
</tr>
<tr>
<td>184.76</td>
<td>0.8</td>
</tr>
</tbody>
</table>

de Kruif 1980
TABLE 4.1.1.52.1 (Continued)

de Kruif 1980
torsion-, weighing effusion

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>186.22</td>
<td>0.9</td>
</tr>
<tr>
<td>187.54</td>
<td>1.0</td>
</tr>
<tr>
<td>25.0</td>
<td>3.7 × 10⁻¹⁰</td>
</tr>
</tbody>
</table>

ΔH_{subl}/(kJ mol⁻¹) = 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-dibenzoanthracene, a,a′-dibenzoanthracene, dinaphthantracene
Chemical Name: dibenz[a,j]anthracene
CAS Registry No: 58-70-3
Molecular Formula: C_{22}H_{14}
Molecular Weight: 278.346
Melting Point (°C): 197.5 (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  222.8 (Ruelle & Kesselring 1997)
  299.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 0.0203 (mp at 197.5°C)
Water Solubility (g/m^3 or mg/L at 25°C or as indicated):
  0.012 (27°C, 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 (Pa at 25°C):
Henry’s Law Constant (Pa m^3/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
  7.19 (calculated-fragment const., Yalkowsky et al. 1983)
  7.11 (calculated-MCI χ 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 ± 0.19, 6.44 ± 0.75 (HPLC-k′ correlation: ODS column; Diol column, Helweg et al. 1997; quoted, Nielsen et al. 1997)
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF:
Sorption Partition Coefficient, log K_{OC}:
  6.58 (humic acid, HPLC-k′ correlation, Nielsen et al. 1997)
Environmental Fate Rate Constants, k or Half-Lives, 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: C_{22}H_{14}
Molecular Weight: 278.346
Melting Point (°C):
  270–271 (Weast 1982–83)
Boiling Point (°C):
  290–300 (sublimation, Weast 1982–83)
Density (g/cm³ at 20°C):
  299.9  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
  35.19  (Chickos et al. 1999)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
  55.22, 44.0  (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
  0.00395 (mp at 270°C)

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°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 × 10^{-13}* (effusion method, De Kruif 1980)
log (P/Pa) = 12.725 – 8260/(T/K); temp range 444–566 K (Antoine eq., Stephenson & Malanowski 1987)
1.19 × 10^{-12}* (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 170–210°C, Oja & Suuberg 1998)
log (P/Pa) = 35.823 – 18867/(T/K); temp range 443–483 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)

Henry’s Law Constant (Pa m³/mol):

Octanol/Water Partition Coefficient, log $K_{\text{OW}}$:
  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 $K_{\text{OA}}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log $K_{\text{OC}}$:

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_{1/2}$:

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

\[
\begin{align*}
\log P &= A - \frac{B}{T/K} \quad (1) \\
\ln P &= A - \frac{B}{T/K} \\n\log P &= A - \frac{B}{C + t/°C} \quad (2) \\
\ln P &= A - \frac{B}{C + t/°C} \\
\log P &= A - \frac{B}{C + T/K} \\
\log P &= A - \frac{B}{T/K} - C \cdot \log (T/K) \quad (4)
\end{align*}
\]

<table>
<thead>
<tr>
<th>de Kruif 1980</th>
<th>Oja &amp; Suuberg 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>torsion-, weighing effusion</td>
<td>Knudsen effusion</td>
</tr>
<tr>
<td>(t/°C)</td>
<td>(P/Pa)</td>
</tr>
<tr>
<td>220.51</td>
<td>0.1</td>
</tr>
<tr>
<td>229.8</td>
<td>0.2</td>
</tr>
<tr>
<td>235.4</td>
<td>0.3</td>
</tr>
<tr>
<td>239.45</td>
<td>0.4</td>
</tr>
<tr>
<td>242.63</td>
<td>0.5</td>
</tr>
<tr>
<td>245.27</td>
<td>0.6</td>
</tr>
<tr>
<td>247.51</td>
<td>0.7</td>
</tr>
<tr>
<td>249.47</td>
<td>0.8</td>
</tr>
<tr>
<td>251.22</td>
<td>0.9</td>
</tr>
<tr>
<td>252.79</td>
<td>1.0</td>
</tr>
<tr>
<td>25.0</td>
<td>(T/K)</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>(\Delta H_{\text{subl}}/(kJ \cdot mol^{-1}) = 155.0)</td>
<td>for temp range 443–483 K</td>
</tr>
<tr>
<td>(\Delta H_{\text{subl}}/(kJ \cdot mol^{-1}) = 155.9)</td>
<td></td>
</tr>
</tbody>
</table>

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: C_{24}H_{12}
Molecular Weight: 300.352
Melting Point (°C):
437.4 (Lide 2003)
Boiling Point (°C):
525 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)
Density (g/cm³ at 25°C):
1.371 (Lide 2003)
Molar Volume (cm³/mol):
244.8 (Ruelle & Kesselring 1997)
219.1 (25°C, calculated-density)
292.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
19.202 (Ruelle & Kesselring 1997)
19.2 (exptl., Chickos et al. 1999)
Entropy of Fusion, ΔS_{fus} (J/mol K):
27.02, 42.8 (exptl., calculated-group additivity method, Chickos et al. 1999)
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 8.99 × 10⁻⁵ (mp at 437.4°C)
Water Solubility (g/m³ or mg/L at 25°C):
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°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):
log (P/mmHg) = 12.62 − 7675/(T/K); temp range 160–240°C (Knudsen effusion method, Hoyer & Peperle 1958)
1.95 × 10⁻¹⁰ (Knudsen effusion method, extrapolated, Murray et al. 1974)
log (P/atm) = 9.110 − 7100/(T/K); temp range 427–510 K (Knudsen effusion method, Murray et al. 1974)
2.00 × 10⁻¹⁰ (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_s/kPa) = 11.157 − 7100/(T/K); temp range 427–510 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_s/kPa) = 11.157 − 7100/(T/K); temp range 427–510 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P_s/kPa) = 8.886 − 5764/(T/K); temp range not specified (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
log (P_s/kPa) = 8.318 − 5362/(T/K); temp range not specified (liquid, Antoine eq.-III, Stephenson & Malanowski 1987)
2.89 × 10⁻¹⁰ (gas saturation, extrapolated-Antoine eq. derived from exptl. data, temp range 148–231°C, Oja & Suuberg 1998)
log (P/Pa) = 31.72 − 16006/(T/K); temp range 421–504 K (Antoine eq., Knudsen effusion, Oja & Suuberg 1998)
2.55 × 10⁻⁸ (supercooled liquid P_L, calibrated GC-RT correlation, Lei et al. 2002)
log (P_L/Pa) = −5446/(T/K) + 10.67; ΔH_{vap.} = −104.2 kJ·mol⁻¹ (GC-RT correlation, Lei et al. 2002)
Henry’s Law Constant (Pa m³/mol at 25°C):

Octanol/Water Partition Coefficient, log \( K_{ow} \):
- 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-\( K_{oc} \), Broman et al. 1991)
- 6.50 (Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log \( K_{oc} \):
- 7.80 (Baltic Sea particulate field samples, concn distribution-GC/MS, Broman et al. 1991)
- 6.50 (predicted dissolved log \( K_{oc} \), Broman et al. 1991)

Environmental Fate Rate Constants, \( k \) or Half-Lives, \( t_{1/2} \):

Half-Lives in the Environment:
- Soil: mean \( t_{1/2} \) = 16.5 yr for Luddington soil (Wild et al. 1991).

### TABLE 4.1.155.1
Reported vapor pressures of coronene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>effusion</strong></td>
<td><strong>Knudsen effusion</strong></td>
<td><strong>Knudsen effusion</strong></td>
</tr>
<tr>
<td>( t/\degree C )</td>
<td>( P/Pa )</td>
<td>( t/\degree C )</td>
</tr>
<tr>
<td>data presented by</td>
<td>data presented by</td>
<td>147.9</td>
</tr>
<tr>
<td>eq. 1</td>
<td>eq. 1</td>
<td>163.6</td>
</tr>
<tr>
<td>A</td>
<td>A</td>
<td>178.1</td>
</tr>
<tr>
<td>B</td>
<td>B</td>
<td>196.9</td>
</tr>
<tr>
<td>for temp range 160–240°C</td>
<td>for temp range 427–510 K</td>
<td>109.9</td>
</tr>
<tr>
<td>( \Delta H_{sub}/(kJ/mol) ) = 147.0</td>
<td>25.0</td>
<td>2.0 × 10⁻¹⁰</td>
</tr>
<tr>
<td>mp/\degree C</td>
<td>~440</td>
<td>extrapolated</td>
</tr>
<tr>
<td>( \Delta H_{sub}/(kJ/mol) ) = 135.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>at av. temp measurements</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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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: C₁₈H₁₁Cl₃
Molecular Weight: 333.639
Melting Point (°C): 92 (Dickhut et al. 1994)
Boiling Point (°C): 
Density (g/cm³): 
Molar Volume (cm³/mol): 335.9 (calculated-Le Bas method at normal boiling point)
Heat of Fusion, ΔHₙₚ (kJ/mol):
Entropy of Fusion, ΔSₙₚ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₙₚ = 56 J/mol K), F: 0.22 (mp at 92°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
3.8 × 10⁻⁴; 3.37 × 10⁻⁴ (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)
1.01 × 10⁻⁴, 6.56 × 10⁻⁴, 8.56 × 10⁻⁴ (5, 25, 30°C, generator column-GC, Dickhut et al. 1994)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₐw:
Octanol/Air Partition Coefficient, log Kₐa:
Bioconcentration Factor, log BCF or log Kₕ:
Sorption Partition Coefficient, log Kₐc:
Environmental Fate Rate Constants, k and Half-Lives, t₁/₂:
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: C₁₈H₁₁Cl₄
Molecular Weight: 368.084
Melting Point (°C):
   114 (Dickhut et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   356.8 (calculated-Le Bas method at normal boiling point)
Heat of Fusion, ΔHₙₑₜ (kJ/mol):
Entropy of Fusion, ΔSₙₑₜ (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSₙₑₜ = 56 J/mol K), F: 0.134 (m.p at 114°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   1.79 × 10⁻⁴; 7.91 × 10⁻⁵ (exptl. mean by generator column-GC method; calculated-TSA, Dickhut et al. 1994)
   5.91 × 10⁻⁵, 1.74 × 10⁻⁴, 4.07 × 10⁻⁴ (5, 25, 40°C, generator column-GC, Dickhut et al. 1994)

Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₐₗₘ:\nOctanol/Air Partition Coefficient, log Kₐₘ:\nBioconcentration Factor, log BCF or log K₉:\nSorption Partition Coefficient, log Kₐₗ:\nEnvironmental Fate Rate Constants, k and Half-Lives, tₜ:\nHalf-Lives in the Environment:
4.1.3 POLYCHLORINATED NAPHTHALENES

4.1.3.1 1-Chloronaphthalene

Common Name: 1-Chloronaphthalene
Synonym: PCN-1, α-chloronaphthalene
Chemical Name: 1-chloronaphthalene
CAS Registry No: 90-13-1
Molecular Formula: C₁₀H₇Cl
Molecular Weight: 162.616

Melting Point (°C):
-2.5 (Lide 2003)

Boiling Point (°C):
259 (Lide 200)

Density (g/cm³):
1.1938 (20°C, Weast 1982–83; Windholz 1983; Budavari 1989)
1.188 (25°C, Lide 2003)

Molar Volume (cm³/mol):
136.2 (20°C, calculated-density)
168.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔHₘₙ (kJ/mol):

Entropy of Fusion, ΔSₘₙ (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):
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°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* (80.6°C, static-Hg manometer, measured range 80.6–269.3°C, Kahlbaum 1898)
133.3* (80.6°C, summary of literature data, temp range 80.6–269.3°C, Stull 1947)
3.055 (extrapolated from Antoine eq., temp range 353–533 K, Stephenson & Malanowski 1987)
2.133 (estimated, Crookes & Howe 1993)
1.2 × 10⁻⁴ (estimated, Alcock et al. 1999)
3.597, 3.84 (calibrated GC-RT correlation, GC-RT correlation, Pₜ, supercooled liquid values, Lei et al. 1999)
log (Pₜ/Pₘ) = –3058/(T/K) + 10.81 (HPLC-RT correlation, Lei et al. 1999)
5.588 (supercooled liquid Pₜ, regression with GC-RT from literature, Lei et al. 1999)
log (Pₜ/Pₘ) = –3054/(T/K) + 9.97; (regression with GC-RT from literature, supercooled liquid, Lei et al. 1999)
6.89* (23.15°C, transpiration method, measured range 289.1–332.3 K, Verevkin 2003)
ln \(\frac{P}{P_0}\) = 299.001/R – 8394.481/R·(T/K) – (73.5/R)·ln[(T/K)/298.15], where \(P_0 = 101.325\) kPa, gas constant \(R = 8.31451\) J·K\(^{-1}\)·mol\(^{-1}\) (vapor pressure eq. from transpiration measurement, temp range 289.1–332.3 K, Verevkin 2003)

Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
- 35.5 (gas stripping-GC, Mackay & Shiu 1981)
- 36.3 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, \(\log K_{ow}\) at 25°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)

\(\log K_{ow} = 0.841 + 940.09/(T/K)\), temp range 5–55°C (temperature dependence HPLC-k’ correlation, Lei et al. 2000)
- 4.06 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, \(\log K_{oa}\) at 25°C or as indicated and reported temperature dependence equations:

\(\log K_{oa} = 58300/(2.303·RT) – 4.40;\) temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, \(\log BCF\) or \(\log K_B\):
- 2.28 (\textit{Cyprinus carpio}, for monochloronaphthalenes, Matsuo 1984; quoted, Crookes & Howe 1993)

Sorption Partition Coefficient, \(\log K_{oc}\):
- 2.97 (estimated for mono-chloronaphthalenes, Crookes & Howe 1993)

Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1/2}\):

### TABLE 4.1.3.1.1
**Reported vapor pressures of 1-chloronaphthalene at various temperatures and the coefficients for the vapor pressure equations**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
<th>t/°C</th>
<th>P/Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>80.6</td>
<td>133.3</td>
<td>80.6</td>
<td>133.3</td>
<td>15.95</td>
<td>3.57</td>
</tr>
<tr>
<td>104.8</td>
<td>666.6</td>
<td>104.8</td>
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(Continued)
### TABLE 4.1.3.1.1 (Continued)

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\[ P = P_0 \exp \left( \frac{A}{\bar{T}} + \frac{B}{\bar{T}^2} \right) \]

\[ \Delta H_v/(kJ \ mol^{-1}) = 62.03 \]

at 298.15 K

---

**FIGURE 4.1.3.1.1** Logarithm of vapor pressure versus reciprocal temperature for 1-chloronaphthalene.

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4.1.3.2 2-Chloronaphthalene

Common Name: 2-Chloronaphthalene
Synonym: PCN-2, β-chloronaphthalene
Chemical Name: 2-chloronaphthalene
CAS Registry No: 91-58-7
Molecular Formula: C_{10}H_{7}Cl
Molecular Weight: 162.616
Melting Point (°C):
58 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
142.9 (71°C, calculated from density, Stephenson & Malanowski 1987)
168.5 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
3.346 (Ruelle & Kesselring 1997)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.474 (mp at 58°C)
Water Solubility (g/m³ or mg/L at 25°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°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 K, Stephenson & Malanowski 1987)
log (P/L/kPa) = 7.8608 – [3021.2/(T/K)]; temp range 400–435 K (Antoine eq., Stephenson & Malanowski 1987)
3.679, 3.84 (supercooled liquid values P_t: calibrated GC-RT correlation, GC-RT correlation, Lei et al. 1999)
log (P/L/Pa) = –3054/(T/K) + 10.81 (GC-RT correlation, supercooled liquid, Lei et al. 1999)
2.526 (supercooled liquid P_t, regression with GC-RT data from literature, Lei et al. 1999)
log (P/L/Pa) = –3054/(T/K) + 9.97 (regression with GC-RT data from literature, Lei et al. 1999)
ln (P/P^o) = 301.255/R – 87496.950/R·(T/K) – (39.5/R)·ln[(T/K)/298.15], where P^o = 101.325 kPa, gas constant R = 8.31451 J·K⁻¹·mol⁻¹ (vapor pressure eq. from transpiration measurement, solid, temp range 280.2–330.7 K, Verevkin 2003)
53.71* (59.05°C, transpiration method, measured range 332.2–362.2 K, Verevkin 2003)
ln (P/P^o) = 294.501/R – 84197.803/R·(T/K) – (73.5/R)·ln[(T/K)/298.15], where P^o = 101.325 kPa, gas constant R = 8.31451 J·K⁻¹·mol⁻¹ (vapor pressure eq. from transpiration measurements, liquid, temp range 332.2–362.2 K, Verevkin 2003)

Henry’s Law Constant (Pa·m³/mol at 25°C):
31.9 (gas stripping-GC, Mackay & Shiu 1981)
33.5 (gas stripping-GC, Shiu & Mackay 1997)
Octanol/Water Partition Coefficient, log $K_{OW}$ at 25°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)
- 4.6024 (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)

\[ \log K_{OW} = 0.821 + \frac{924.42}{(T/K)}, \text{ temp range 5–55°C (temperature dependence HPLC-}k'\text{ correlation, Lei et al. 2000)} \]

Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°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 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)

\[ \log K_{OA} = \frac{58000}{(2.303 \cdot RT)} – 4.40; \text{ temp range 10–50°C (GC-RT correlation, Su et al. 2002)} \]

Bioconcentration Factor, log BCF or log $K_B$:

- 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-$K_{OW}$ and $S_p$, 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-$K_{OW}$, Lu et al. 1999)

Sorption Partition Coefficient, log $K_{OC}$:

- 2.97 (estimated for monochloronaphthalenes, Crookes & Howe 1993)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

- Volatilization:
- Photolysis:
- Photooxidation:
- Hydrolysis: laboratory determined hydrolysis rate constant $k = (9.5 \pm 2.8) \times 10^{-6} \text{ h}^{-1}$ at neutral conditions, calculated $t_{1/2} = 8.3 \text{ yr}$ at pH 7 (Ellington et al. 1988).
- Biodegradation:
- Biotransformation:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

\[ \log k_1 = 2.83 \text{ d}^{-1}; \log k_2 = -0.51 \text{ d}^{-1} \text{ (guppy, Gobas et al. 1989)} \]

Half-Lives in the Environment:

- Air:
- Surface water:
- Ground water:
- Sediment:
- Soil: experimentally measured abiotic disappearance $t_{1/2} = 11.3 \text{ d}$ in two different soil types, a Captina silt loam (Typic Fragiudult) and McLaurin sandy loam (Typic Paleudults) (Anderson et al. 1991).
- Biota: $t_{1/2} = 2.3 \text{ d}$ (female guppies, Opperhuizen et al. 1985, quoted, Crookes & Howe 1993)
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$\Delta H_v/(kJ \text{ mol}^{-1}) = 62.3 \pm 1.1$

at 298.15 K
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: C_{10}H_{6}Cl_{2}
Molecular Weight: 197.061
Melting Point (°C):
36  (Lide 2003)
Boiling Point (°C):
295.6  (Lide 2003)
Density (g/cm³): 1.3147 (49°C, Weast 1982–83; Lide 2003)
Molar Volume (cm³/mol):
156  (Ruelle & Kesselring 1997)
189.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.78 (mp at 36°C)
Water Solubility (g/m³ or mg/L at 25°C):
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°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 (P_L/Pa) = −3172/(T/K) + 10.18; (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.301  (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
log (P_L/Pa) = −3172/(T/K) + 10.11 (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{OW} at 25°C and the reported temperature dependence equations:
4.40  (HPLC-RT correlation, Opperhuizen et al. 1985)
4.66  (selected, Alcock et al. 1999)
4.60; 4.45  (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
log K_{OW} = 1.064 + 1060.21/(T/K), temp range 5–55°C (temperature dependence HPLC-k’ correlation, Lei et al. 2000)
4.69  (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log K_{OA} at 25°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 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
log K_{OA} = 66000/(2.303·RT) − 4.800; temp range 10–50°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 BCF or log K_{B}:
3.40  (fish, Opperhuizen et al. 1985)
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k and Half-Lives, t½:
Half-Lives in the Environment:
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: C_{10}H_{6}Cl_{2}
Molecular Weight: 197.061
Melting Point (°C):
   67.5  (Lide 2003)
Boiling Point (°C):
   288  (Lide 2003)
Density (g/cm³): 156.0  (Ruelle & Kesselring 1997)
   189.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.383 (mp at 288°C)
Water Solubility (g/m³ or mg/L at 25°C):
   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°C and reported temperature dependence equations):
   0.173  (estimated, Crookes & Howe 1993)
   9.98 × 10⁻⁶  (estimated, Alcock et al. 1999)
   0.428; 0.416 (supercooled liquid P_L; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
log (P_L/Pa) = –3067/(T/K) + 9.92 (GC-RT correlation, supercooled liquid, Lei et al. 1999)
   0.353  (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
log (P_L/Pa) = –3067/(T/K) + 10.17 (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow} at 25°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 K_{ow} = 1.269 + 1049.8/(T/K), temp range 5–55°C (temperature dependence HPLC-k’ correlation, Lei et al. 2000)
   4.56  (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log K_{oa} at 25°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  (10, 20, 30, 40, 50°C, generator column-GC/MS, Harner & Bidleman 1998)
\[
\log K_{OA} = -3.97 + \frac{3248}{T/K}, \text{ temp range: 10–50°C (generator column-GC/MS, Harner & Bidleman 1998)}
\]
\[
6.78; 6.91 \text{ (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)}
\]

**Bioconcentration Factor, log BCF or log \(K_B\):**

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<th>Value</th>
<th>Reference</th>
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<tr>
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<td>((\text{Opperhuizen et al. 1985}))</td>
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<td>((\text{Opperhuizen et al. 1985}))</td>
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<td>((\text{guppies: whole fish, fish lipid, Gobas et al. 1987}))</td>
</tr>
<tr>
<td>3.75</td>
<td>((\text{rainbow trout, Oliver &amp; Niimi 1984; Oliver 1987}))</td>
</tr>
<tr>
<td>5.18</td>
<td>((\text{guppy, lipid-weight based, Gobas et al. 1989}))</td>
</tr>
<tr>
<td>3.36; 4.63</td>
<td>((\text{quoted means; calculated-(K_{OW}) and (S_p), Banerjee &amp; Baughman 1991}))</td>
</tr>
<tr>
<td>3.75</td>
<td>((\text{((\text{Oncorhynchus mykiss, under flow-through condition, quoted Devillers et al. 1996}))}))</td>
</tr>
<tr>
<td>3.36</td>
<td>((\text{((\text{Poecilia reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996}))}))</td>
</tr>
</tbody>
</table>

**Sorption Partition Coefficient, log \(K_{OC}\):**

**Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1/2}\):**

**Volatilization:**

**Photolysis:**

**Photooxidation:** rate constant \(k = 5.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}\) for the gas-phase reactions with OH radical at \(298 \pm 2 \text{ K (Atkinson 1989)}\).

**Hydrolysis:**

**Biodegradation:**

**Biotransformation:**

**Bioconcentration and Uptake and Elimination Rate Constants (\(k_1\) and \(k_2\)):**

\[
\begin{align*}
k_1 & = 1.2 \times 10^3 \text{ d}^{-1}; \\
& k_2 = 1.1 \times 10^{-1} \text{ d}^{-1} \text{ (guppies, Opperhuizen et al. 1985)}
\end{align*}
\]

\[
\begin{align*}
\log k_1 & = 3.04 \text{ d}^{-1}; \\
& \log k_2 = -0.96 \text{ d}^{-1} \text{ (guppy, Gobas et al. 1989)}
\end{align*}
\]

**Half-Lives in the Environment:**

**Biota:** \(t_{1/2} = 6.2 \text{ d (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)}\)
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: C_{10}H_6Cl_2
Molecular Weight: 197.061
Melting Point (°C):
89 (Weast 1982-83; Lide 2003)
Boiling Point (°C):
sublimation (Lide 2003)
Density (g/cm³):

Molar Volume (cm³/mol):
156.0 (Ruelle & Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.236 (mp at 89°C)
Water Solubility (g/m³ or mg/L at 25°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°C and the reported temperature dependence equation):
0.198 (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
log (P_L/Pa) = –3169/(T/K) + 9.93 (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{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 K_{OA}:
Bioconcentration Factor, log BCF or log K_{bi}:
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 (P. reticulata, under static and semi-static conditions, quoted, Devillers et al. 1996)
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
k_1 = 9.8 \times 10^2 \, d^{-1}; k_2 = 1.6 \times 10^{-1} \, d^{-1} \text{ (guppies, Opperhuizen et al. 1985)}
log k_1 = 2.97 \, d^{-1}; log k_2 = -0.80 \, d^{-1} \text{ (guppy, Gobas et al. 1989)}
Half-Lives in the Environment:
Biota: elimination t_{1/2} = 4.3 \, d \text{ (guppies, Opperhuizen et al. 1985; Crookes & Howe 1993)}
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: C_{10}H_{6}Cl_{2}
Molecular Weight: 197.061
Melting Point (°C):
  120  (Weast 1982-83; Ruelle & Kesselring 1997; Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
  156.0  (Ruelle & Kesselring 1997)
  189.4  (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.117 (mp at 120°C)
Water Solubility (g/m³ or mg/L at 25°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°C and the reported temperature dependence equation):
  0.333  (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
    log (P_L/Pa) = –3169/(T/K) + 10.15 (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{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 K_{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 K_{OC}:
Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:
  Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):
    k_1 = 1.6 × 10^3 d^{-1};  k_2 = 1.4 × 10^{-1} d^{-1} (guppies, Opperhuizen et al. 1985)
    log k_1 = 3.05 d^{-1};  log k_2 = –0.85 d^{-1} (guppy, Gobas et al. 1989)
  Half-Lives in the Environment:
    Biota: elimination t_{1/2} = 5.1 d (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)
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: C_{10}H_{6}Cl_{2}
Molecular Weight: 197.061
Melting Point (°C): 115 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
156.0 (Ruelle & Kesselring 1997)
189.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.131 (mp at 115°C)
Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equation):
0.344 (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
log (P_l/P_a) = –3169/(T/K) + 10.16 (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
4.81 (HPLC-RT correlation, Opperhuizen et al. 1985)
4.56 (shake flask-GC, Opperhuizen 1987)
Octanol/Air Partition Coefficient, log K_{oa} at 25°C and reported temperature dependence equation:
7.28, 6.95, 6.38, 6.08, 5.85 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
log K_{oa} = 65400/(2.303·RT) – 4.80; temp range 10–50°C (GC-RT correlation, Su et al. 2002)
Bioconcentration Factor, log BCF or log K_{bc}:
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 K_{oc}:
Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:
Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 1.6 \times 10^3$ d⁻¹; $k_2 = 1.4 \times 10^{-1}$ d⁻¹ (guppies, Opperhuizen et al. 1985)
log $k_1 = 3.08$ d⁻¹; log $k_2 = -0.85$ d⁻¹ (guppy, Gobas et al. 1989)
Half-Lives in the Environment:
Biota: depuration $t_{1/2} = 5.1$ d (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)
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: C\textsubscript{10}H\textsubscript{5}Cl\textsubscript{3}
Molecular Weight: 231.506
Melting Point (°C): 81–84 (Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
210.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH\textsubscript{v} (kJ/mol):
Enthalpy of Sublimation, ΔH\textsubscript{subl} (kJ/mol):
Enthalpy of Fusion, ΔH\textsubscript{ fus} (kJ/mol):
Entropy of Fusion, ΔS\textsubscript{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS\textsubscript{ fus} = 56 J/mol K), F:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.071; 0.0652 (supercooled liquid P\textsubscript{L}; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
log (P\textsubscript{L}/Pa) = –3551/(T/K) + 10.76 (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.0791 (supercooled liquid P\textsubscript{L}, regression with GC-RT data from literature, Lei et al. 1999)
log (P\textsubscript{L}/Pa) = –3485/(T/K) + 10.59 (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
Octanol/Water Partition Coefficient, log K\textsubscript{OW}:
Octanol/Air Partition Coefficient, log K\textsubscript{OA} at 25°C and reported temperature dependence equation:
8.24, 7.85, 7.30, 6.91, 6.63 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
log K\textsubscript{OA} = 73200/(2.303·RT) – 5.20; temp range 10–50°C (GC-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\textsubscript{B}:
Sorption Partition Coefficient, log K\textsubscript{OC}:
Environmental Fate Rate Constants, k and Half-Lives, t\textsubscript{1/2}:
Half-Lives in the Environment:
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: C_{10}H_{5}Cl_{3}
Molecular Weight: 231.506
Melting Point (°C): 113 (Crookes & Howe 1993)
Boiling Point (°C): 274
Density (g/cm³):
Molar Volume (cm³/mol):
168.9 (Ruelle & Kesselring 1997)
210.3 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.137 (mp at 113°C)
Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equation):
0.127 (estimated, Crookes & Howe 1993)
7.10 × 10⁻⁶ (estimated, Alcock et al. 1999)
0.114 (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
log (P_L/P_a) = −3485/(T/K) + 10.74 (regression with GC-RT from literature, Lei et al. 1999)
0.0778 – P_S, 0.359 – P_L (estimated for trichloronaphthalenes, Kaupp & McLachlan 1999)
Henry's Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{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 K_{oa}:
Bioconcentration Factor, log BCF or log K_{bi}:
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-K_{ow} and solubility, Banerjee & Baughman 1991)
4.43 (Poecilia reticulata, under static and semi-static conditions, Devillers et al. 1996)
Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):

$k_1 = 2.3 \times 10^3$ d$^{-1}$; $k_2 = 8.4 \times 10^{-2}$ d$^{-1}$ (guppy, Opperhuizen et al. 1985)

$k_1 = 1.7 \times 10^3$ d$^{-1}$ (estimated, Opperhuizen et al. 1985)

$log k_1 = 3.14$ d$^{-1}$; $log k_2 = -1.64$ d$^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

Biota: $t_{1/2} = 8.3$ d (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)
4.1.3.10 1,2,3,4-Tetrachloronaphthalene

![structure](image)

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: C_{10}H_{4}Cl_{4}
Molecular Weight: 265.951
Melting Point (°C):
199 (Lide 2003)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
181.8 (Ruelle & Kesselring 1997)
231.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.0196 (mp at 199°C)

Water Solubility (g/m³ or mg/L at 25°C):
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°C and reported temperature dependence equations):
0.0197; 0.0173 (supercooled liquid P_{L}; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
log (P_{L}/Pa) = -3825/(T/K) + 11.12; (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.0162 (supercooled liquid P_{L}, regression with GC-RT from literature, Lei et al. 1999)
log (P_{L}/Pa) = -3825/(T/K) + 10.96 (regression with GC-RT from literature, Lei et al. 1999)
0.00536 – P_{S}; 0.0975 – P_{L} (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{OW} at 25°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 K_{OW} = 1.832 + 1347.46/(T/K), temp range 5–55°C (temperature dependence HPLC-k′ correlation, Lei et al. 2000)
5.91 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log K_{OA} at 25°C or as indicated and reported temperature dependence equation:
9.03, 8.59, 8.05, 7.59, 7.26 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
log K_{OA} = 79500/(2.303-RT) – 5.60; temp range 10–50°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 BCF or log $K_B$:

- $3.94$ (Cyprinus carpio, Matuo 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 $K_{OC}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_\frac{1}{2}$:

- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_1 = 3.3 \times 10^3$ d$^{-1}$; $k_2 = 9.9 \times 10^{-2}$ d$^{-1}$ (guppy, Opperhuizen et al. 1985)
  - $k_1 = 1.3 \times 10^3$ d$^{-1}$ (estimated, Opperhuizen et al. 1985)
  - log $k_1 = 3.70$ d$^{-1}$; log $k_2 = -1.08$ d$^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:

- Biota: $t_\frac{1}{2} = 7$ d (guppies, Opperhuizen et al. 1985; quoted, Crookes & Howe 1993)
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: C_{10}H_{4}Cl_{4}
Molecular Weight: 265.951
Melting Point (°C): 141 (Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
231.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0728 (mp at 141°C)

Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
0.0203; 0.0179 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
\[ \log (P_L/Pa) = -3836/(T/K) + 11.17; \] (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.0205 (supercooled liquid P_L, regression with GC-RT data from literature, Lei et al. 1999)
\[ \log (P_L/Pa) = -3800/(T/K) + 11.06 \] (regression with GC-RT data from literature, Lei et al. 1999)

Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow}:
5.78 (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log K_{oa} at 25°C or as indicated and reported temperature dependence equation:
8.98, 8.55, 8.00, 7.55, 7.22 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
\[ \log K_{oa} = 79100/(2.303·RT) – 5.60; \] temp range 10–50°C (GC-RT correlation, Su et al. 2002)
8.29; 8.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_{bi}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k and Half-Lives, t_\text{½}:
Half-Lives in the Environment:
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: C\textsubscript{10}H\textsubscript{4}Cl\textsubscript{4}
Molecular Weight: 265.951
Melting Point (°C): 179 (Crookes & Howe 1993)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
  181.8 (Ruelle & Kesselring 1997)
  231.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.0308 (mp at 179°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
  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°C and reported temperature dependence equation):
  0.0480 (estimated, Crookes & Howe 1993)
  2.70 \times 10^{-6} (estimated, Alcock et al. 1999)
  0.0415 (supercooled liquid $P_L$, regression with GC-RT from literature, Lei et al. 1999)
  $\log (P_b/P_a) = -3800/(T/K) + 11.36$ (regression with GC-RT from literature, Lei et al. 1999)
  0.00536 – $P_S$; 0.0975 – $P_L$ (estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol):
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
  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 $K_{\text{oa}}$ at 25°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 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
  $\log K_{\text{oa}} = 75000/(2.303\cdot RT) – 5.40$; temp range 10–50°C (GC-RT correlation, Su et al. 2002)
Bioconcentration Factor, log BCF or log $K_b$:
  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)
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5.81 (guppy, lipid-weight based, Gobas et al. 1989)
4.53; 4.37 (quoted means; calculated-K\textsubscript{OW} and S, Banerjee & Baughman 1991)
4.701, 4.961 (calculated-MCI \chi, calculated-K\textsubscript{OW}, Lu et al. 1999)

Sorption Partition Coefficient, log K\textsubscript{OC}:

Environmental Fate Rate Constants, k and Half-Lives, t\textsubscript{1/2}:
  Bioconcentration and Uptake and Elimination Rate Constants (k\textsubscript{1} and k\textsubscript{2}):  
    k\textsubscript{1} = 7.5 \times 10^2 \text{ d}^{-1}; k\textsubscript{2} = 2.2 \times 10^{-2} \text{ d}^{-1} (guppies, Opperhuizen et al. 1985)
    log k\textsubscript{1} = 2.97 \text{ d}^{-1}; log k\textsubscript{2} = -1.66 \text{ d}^{-1} (guppy, Gobas et al. 1989)

Half-Lives in the Environment:
  Biota: t\textsubscript{1/2} = 30 \text{ d} (guppies, Opperhuizen et al. 1985)
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: C\textsubscript{10}H\textsubscript{4}Cl\textsubscript{4}
Molecular Weight: 265.951
Melting Point (°C): 131 (Crookes & Howe 1993; Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}): 181.8 (Ruelle & Kesselring 1997)
Molar Volume (cm\textsuperscript{3}/mol): 231.2 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \(\Delta H\text{\textsubscript{fus}}\) (kJ/mol): 231.2 (calculated-Le Bas method at normal boiling point)
Entropy of Fusion, \(\Delta S\text{\textsubscript{fus}}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S\text{\textsubscript{fus}} = 56\) J/mol K), F:\ 0.0912 (mp at 131°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
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°C and reported temperature dependence equation):
\[0.0208 \quad \text{(supercooled liquid P}_L\text{, regression with GC-RT from literature, Lei et al. 1999)}\]
\[\log (P_L/P_a) = -3800/(T/K) + 11.07 \quad \text{(regression with GC-RT from literature, Lei et al. 1999)}\]
\[0.00536 - P_S; 0.0975 - P_L \quad \text{(estimated for tetrachloronaphthalenes, Kaupp & McLachlan 1999)}\]
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol):
Octanol/Water Partition Coefficient, log \(K\text{\textsubscript{OW}}\):
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 \(K\text{\textsubscript{OA}}\) at 25°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 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
\[\log K_OA = 79100/(2.303\cdot RT) - 5.60; \text{temp range 10–50°C (GC-RT correlation, Su et al. 2002)}\]
Bioconcentration Factor, log BCF or log \(K\text{\textsubscript{B}}\):
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-\(K\text{\textsubscript{OW}}\), Lu et al. 1999)
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:
- Bioconcentration and Uptake and Elimination Rate Constants ($k_1$ and $k_2$):
  - $k_1 = 1.2 \times 10^3 \text{ d}^{-1}$; $k_2 = 4.5 \times 10^{-2} \text{ d}^{-1}$ (guppies, Opperhuizen et al. 1985)
  - $k_1 = 1.4 \times 10^3 \text{ d}^{-1}$ (fish, Opperhuizen 1986)
  - $\log k_1 = 3.10 \text{ d}^{-1}$; $\log k_2 = -1.35 \text{ d}^{-1}$ (guppy, Gobas et al. 1989)

Half-Lives in the Environment:
- Biota: $t_{1/2} = 15.5 \text{ d}$ (guppies, Opperhuizen et al. 1985)
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: C_{10}H_{3}Cl_{5}
Molecular Weight: 300.396
Melting Point (°C):
147 (Crookes & Howe 1993; Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
252.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, ΔH_v (kJ/mol):
Enthalpy of Sublimation, ΔH_subl (kJ/mol):
Enthalpy of Fusion, ΔH_fus (kJ/mol):
Entropy of Fusion, ΔS_fus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_fus = 56 J/mol K), F: 0.0635 (mp at 147°C)
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):
0.00562; 0.00475 (supercooled liquid P_L; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
log (P_L/Pa) = – 4123/(T/K) + 11.58; (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.0055 (supercooled liquid P_L, regression with GC-RT data from literature, Lei et al. 1999)
log (P_L/Pa) = –4116/(T/K) + 11.55 (regression with GC-RT data from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log K_{ow} at 25°C and the reported temperature dependence equations:
7.0; 6.27 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
log K_{ow} = 2.166 + 1446.69/(T/K), temp range 5–55°C (temperature dependence HPLC-k correlation, Lei et al. 2000)
Octanol/Air Partition Coefficient, log K_{oa} at 25°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 (10, 20, 30, 40, 50°C, generator column-GC/MS, Harner & Bidleman 1998)
log K_{oa} = –6.63 + 4629/(T/K), temp range: 10–50°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 BCF or log K_{bc}:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:
Half-Lives in the Environment:
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: C_{10}H_{3}Cl_{5}
Molecular Weight: 300.396
Melting Point (°C):
171 (Crookes & Howe 1993; Järnberg et al. 1994)
Boiling Point (°C):
313 (estimated, Crookes & Howe 1993)
Density (g/cm³):
252.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):
Entropy of Fusion, ΔS_{ fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.0369 (mp at 171°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.0073 (estimated, Crookes & Howe 1993)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
4.266 × 10^{-3} (estimated, Crookes & Howe 1993)
2.40 × 10^{-6} (estimated, Alcock et al. 1999)
0.00696; 0.00593 (supercooled liquid P_{ L}; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
log (P_{ L}/Pa) = -4082/(T/K) + 11.53 (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.00798 (supercooled liquid P_{ L}, regression with GC-RT data from literature, Lei et al. 1999)
log (P_{ L}/Pa) = -4082/(T/K) + 11.71 (regression with GC-RT data from literature, Lei et al. 1999)
0.0–133 – P_{ S}; 0.0277 – P_{ L} (estimated for pentachloronaphthalenes, Kaupp & McLachlan 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ 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 K_{ OA} at 25°C or as indicated and reported temperature dependence equations:
8.73 (generator-column-GC, Harner & Bidleman 1998)
log K_{ OA} = -6.02 + 4394/(T/K); temp range: 10–50°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 K_{ bi}:
4.23 (selected, Hawker 1990)
Sorption Partition Coefficient, log K_{ OC}:
4.36 (estimated, Crookes & Howe 1993)
Environmental Fate Rate Constants, k and Half-Lives, t_{ 1/2}:
Half-Lives in the Environment:
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: C\textsubscript{10}H\textsubscript{3}Cl\textsubscript{5}
Molecular Weight: 300.396
Melting Point (°C): 174–176 (Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
252.1 (calculated-Le Bas method at normal boiling point)
Enthalpy of Vaporization, $\Delta H_v$ (kJ/mol):
Enthalpy of Sublimation, $\Delta H_{subl}$ (kJ/mol):
Enthalpy of Fusion, $\Delta H_{fus}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{fus}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
Vapor Pressure (Pa at 25°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)
$\log (P_L/Pa) = -4204/(T/K) + 11.70$ (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.00428 (supercooled liquid $P_L$, regression with GC-RT data from literature, Lei et al. 1999)
$\log (P_L/Pa) = -4116/(T/K) + 11.44$ (regression with GC-RT data from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
Octanol/Water Partition Coefficient, log $K_{ow}$ at 25°C and the temperature dependence equations:
6.80; 6.13 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
$\log K_{ow} = 2.305 + 1431.02/(T/K)$, temp range 5–55°C (temperature dependence HPLC-$k'$ correlation, Lei et al. 2000)
6.46 (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log $K_{oa}$ at 25°C or as indicated and reported temperature dependence equations:
9.97, 9.44, 8.86, 8.34, 7.96 (10, 20, 30, 40, 50°C, generator column-GC/MS, Harner & Bidleman 1998)
$\log K_{oa} = -6.59 + 4684/(T/K)$; temp range: 10–50°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 BCF or log $K_b$:
Sorption Partition Coefficient, log $K_{oc}$:
Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:
Half-Lives in the Environment:
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: C_{10}H_{2}Cl_{6}
Molecular Weight: 334.842
Melting Point (°C):
194 (Crookes & Howe 1993)
164–166 (Järnberg et al. 1994)
Boiling Point (°C):
331 (estimated, Crookes & Howe 1993)
Density (g/cm³):
Molar Volume (cm³/mol):
273.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.022 (mp at 194°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.00011 (estimated, Crookes & Howe 1993)
Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
9.47 × 10⁻⁴ (estimated, Crookes & Howe 1993)
5.30 × 10⁻⁸ (estimated, Alcock et al. 1999)
0.00134 (supercooled liquid P_L, regression with GC-RT data from literature, Lei et al. 1999)
\log (P_L/P_a) = –4432/(T/K) + 11.99 (regression with GC-RT data from literature, Lei et al. 1999)
0.000257 – P_S; 0.00809 – P_L (estimated for hexachloronaphthalenes, Kaupp & McLachlan 1999)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
7.58 (estimated, Crookes & Howe 1993, quoted, Alcock et al. 1999)
Octanol/Air Partition Coefficient, log K_{OA} at 25°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 (20, 30, 40, 50°C, generator column-GC/MS, Harner & Bidleman 1998)
\log K_{OA} = –6.77 + 4393/(T/K); temp range: 20–50°C (generator column-GC/MS, Harner & Bidleman 1998)
10.02 (value for hexachloronaphthalenes, Kaupp & McLachlan 1999)
Bioconzentration Factor, log BCF or log K_{b}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:
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: C\(_{10}\)H\(_2\)Cl\(_6\)
Molecular Weight: 334.842
Melting Point (°C): 205-206 (Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm\(^3\)):
Molar Volume (cm\(^3\)/mol):
Enthalpy of Vaporization, \(\Delta H_v\) (kJ/mol):
Enthalpy of Sublimation, \(\Delta H_{subl}\) (kJ/mol):
Enthalpy of Fusion, \(\Delta H_{fus}\) (kJ/mol):
Entropy of Fusion, \(\Delta S_{fus}\) (J/mol K):
Fugacity Ratio at 25°C (assuming \(\Delta S_{fus} = 56\) J/mol K), F:
Water Solubility (g/m\(^3\) or mg/L at 25°C):
Vapor Pressure (Pa at 25°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)
\(\log (P_v/P_a) = \frac{-4411}{(T/K)} + 11.97\) (GC-RT correlation, supercooled liquid, Lei et al. 1999)
\(0.00157\) (supercooled liquid \(P_L\), regression with GC-RT from literature, Lei et al. 1999)
\(\log (P_v/P_a) = \frac{-4432}{(T/K)} + 12.06\) (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m\(^3\)/mol at 25°C):
Octanol/Water Partition Coefficient, \(\log K_{ow}\) at 25°C and the temperature dependence equations:
7.70; 6.79 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
\(\log K_{ow} = 2.489 + 1556.37/(T/K)\); temp range 5–55°C (temperature dependence HPLC-k’ correlation, Lei et al. 2000)
6.77 (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, \(\log K_{oa}\) at 25°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 (10, 20, 30, 40, 50°C, generator column-GC/MS, Harner & Bidleman 1998)
\(\log K_{oa} = -7.09 + 5003/(T/K)\); temp range: 10–50°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, \(\log BCF\) or \(\log K_{bf}\):
Sorption Partition Coefficient, \(\log K_{oc}\):
Environmental Fate Rate Constants, \(k\) and Half-Lives, \(t_{1/2}\):
Half-Lives in the Environment:
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: C\textsubscript{10}H\textsubscript{2}Cl\textsubscript{6}
Molecular Weight: 334.842
Melting Point (°C): 234–235 (Järnberg et al. 1994)
Boiling Point (°C): 273.0 (calculated-Le Bas method at normal boiling point)
Density (g/cm\textsuperscript{3}): 273.0 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm\textsuperscript{3}/mol):
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol):
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F:
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):

\[
0.00150; 0.00121 \quad (\text{supercooled liquid } P_L; \text{calibrated GC-RT correlation}; \text{GC-RT correlation, Lei et al. 1999})
\]
\[
\log (P_L/\text{Pa}) = -4411/(T/K) + 11.97 \quad (\text{GC-RT correlation, supercooled liquid, Lei et al. 1999})
\]
\[
0.00157 \quad (\text{supercooled liquid } P_L, \text{regression with GC-RT data from literature, Lei et al. 1999})
\]
\[
\log (P_L/\text{Pa}) = -4432/(T/K) + 12.06 \quad (\text{regression with GC-RT data from literature, Lei et al. 1999})
\]
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol at 25°C):
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
Octanol/Air Partition Coefficient, log $K_{\text{oa}}$ at 25°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 (10, 20, 30, 40, 50°C, generator column-GC/MS, Harner & Bidleman 1998)
\[
\log K_{\text{oa}} = -7.09 + 5003/(T/K); \text{temp range: 10–50°C (generator column-GC/MS, Harner & Bidleman 1998})
\]
9.58; 9.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
Bioconcentration Factor, log BCF or log $K_{\text{bi}}$:
Sorption Partition Coefficient, log $K_{\text{OC}}$:
Environmental Fate Rate Constants, k and Half-Lives, $t_{\frac{1}{2}}$:
Half-Lives in the Environment:
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: C_{10}H_{2}Cl_{6}
Molecular Weight: 334.842
Melting Point (°C): 148–149 (Järnberg et al. 1994)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
   273.0 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{ fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{ fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{ fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C and the reported temperature dependence equations):
   0.00124; 0.0010 (supercooled liquid \( P_L \); calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
   \[ \log \left( \frac{P_L}{Pa} \right) = -4441/(T/K) + 11.99 \] (GC-RT correlation, supercooled liquid, Lei et al. 1999)
   0.00134 (supercooled liquid \( P_L \), regression with GC-RT from literature, Lei et al. 1999)
   \[ \log \left( \frac{P_L}{Pa} \right) = -4432/(T/K) + 11.99 \] (regression with GC-RT from literature, Lei et al. 1999)
Henry’s Law Constant (Pa·m³/mol at 25°C):
Octanol/Water Partition Coefficient, log \( K_{\text{ ow}} \) at 25°C and the reported temperature dependence equations:
   7.50; 6.69 (calibrated HPLC-RT correlation; HPLC-RT correlation, Lei et al. 2000)
   \[ \log K_{\text{ ow}} = 2.413 + 1535.48/(T/K) \] (temp range 5–55°C (temperature dependence HPLC-\( k’ \) correlation, Lei et al. 2000)
   6.87 (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log \( K_{\text{ OA}} \) at 25°C or as indicated and reported temperature dependence equation:
   9.83 (generator column-GC,MS, Harner & Bidleman 1998)
   \[ \log K_{\text{ OA}} = -6.64 + 4909/(T/K) \] (temp range: 20–50°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 BCF or log \( K_B \):
Sorption Partition Coefficient, log \( K_{\text{ OC}} \):
Environmental Fate Rate Constants, k and Half-Lives, \( t_{1/2} \):
Half-Lives in the Environment:
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: C_{10}HCl_{7}
Molecular Weight: 369.287
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
293.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), \( F \):

Water Solubility (g/m³ or mg/L at 25°C):
0.00062 (generator column-GC/ECD, Opperhuizen 1985; quoted, Opperhuizen 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):
5.44 \times 10^{-4} – P_S; 0.00258 – P_L (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)
2.93 \times 10^{-4}, 2.78 \times 10^{-4} (supercooled liquid \( P_L \); calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
\log (P_L/Pa) = -4745/(T/K) + 12.38 (GC-RT correlation, supercooled liquid, Lei et al. 1999)
0.000278 (supercooled liquid \( P_L \), regression with GC-RT from literature, Lei et al. 1999)
\log (P_L/Pa) = -4745/(T/K) + 12.37 (regression with GC-RT from literature, Lei et al. 1999)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \) at 25°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 \( K_{\text{OW}} \) = 2.638 + 1660.82/(T/K); temp range 5–55°C (HPLC-k correlation, Lei et al. 2000)
7.33 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \) at 25°C or as indicated and reported temperature dependence equation:
11.52, 10.96, 10.44, 9.75, 9.28 (10, 20, 30, 40, 50°C, GC-RT correlation, Su et al. 2002)
log \( K_{\text{OA}} \) = 99500/(2.303-RT) – 6.80; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, log BCF or log \( K_b \):
Sorption Partition Coefficient, log \( K_{\text{OC}} \):

Environmental Fate Rate Constants, k and Half-Lives, \( t_{1/2} \):
Half-Lives in the Environment:
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: C₁₀HCl₇
Molecular Weight: 369.287
Melting Point (°C):
194 (Crookes & Howe 1993; Järnberg et al. 1994)
Boiling Point (°C):
348 (estimated, Crookes & Howe 1993)
Density (g/cm³):

Molar Volume (cm³/mol):
293.9 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{ fus} (kJ/mol):

Entropy of Fusion, ΔS_{ fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{ fus} = 56 J/mol K), F: 0.022 (mp at 194°C)
Water Solubility (g/m³ or mg/L at 25°C):
0.00004 estimated, Crookes & Howe 1993; quoted, Alcock et al. 1999)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):
3.73 × 10⁻⁴ (estimated, Crookes & Howe 1993)
2.10 × 10⁻³ (estimated, Alcock et al. 1999)
2.46 × 10⁻⁴ (supercooled liquid P_L, regression with GC-RT from literature, Lei et al. 1999)
log (P_L/Pa) = –4748/(T/K) + 12.31 (regression with GC-RT from literature, Lei et al. 1999)
5.44 × 10⁻⁴ – P_S; 0.00258 – P_L (estimated for heptachloronaphthalenes, Kaupp & McLachlan 1999)

Henry’s Law Constant (Pa·m³/mol):

Octanol/Water Partition Coefficient, log K_{ 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 K_{ OA} at 25°C or as indicated and reported temperature dependence equation:
log K_{ OA} = 99800/(2.303·RT) – 6.80; temp range 10–50°C (GC-RT correlation, Su et al. 2002)

Bioconcentration Factor, log BCF or log K_{ b}:

Sorption Partition Coefficient, log K_{ OC}:

Environmental Fate Rate Constants, k and Half-Lives, t_{ ½}:
Half-Lives in the Environment:
4.1.3.23 Octachloronaphthalene

Common Name: Octachloronaphthalene
Synonym: PCN-75
Chemical Name: octachloronaphthalene
CAS Registry No: 2234-13-1
Molecular Formula: C\textsubscript{10}Cl\textsubscript{8}
Molecular Weight: 403.731
Melting Point (°C): 197.5 (Lide 2003)
Boiling Point (°C): 365 (estimated, Crookes & Howe 1993)
Density (g/cm\textsuperscript{3}):
Molar Volume (cm\textsuperscript{3}/mol):
- 314.8 (calculated-Le Bas method at normal boiling point)
- 233.7 (Ruelle & Kesselring 1997)
Enthalpy of Fusion, (∆H\textsubscript{fus} (kJ/mol):
Entropy of Fusion, (∆S\textsubscript{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ∆S\textsubscript{fus} = 56 J/mol K), F: 0.0203 (mp at 197.5°C)
Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):
- 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°C and reported temperature dependence equations):
- 1.33 × 10\textsuperscript{-4} (estimated, Crookes & Howe 1993)
- 7.50 × 10\textsuperscript{-9} (estimated, Alcock et al. 1999)
- 7.61 × 10\textsuperscript{-3}, 5.60 × 10\textsuperscript{-2} (supercooled liquid P\textsubscript{T}; calibrated GC-RT correlation; GC-RT correlation, Lei et al. 1999)
- log (P\textsubscript{T}/Pa) = −5021/(T/K) + 12.72 (Antoine eq., GC-RT correlation, supercooled liquid, Lei et al. 1999)
- 6.84 × 10\textsuperscript{-5} (supercooled liquid P\textsubscript{T}; regression with GC-RT from literature, Lei et al. 1999)
- log (P\textsubscript{T}/Pa) = −5021/(T/K) + 12.82 (regression with GC-RT from literature, Lei et al. 1999)
- 1.60 × 10\textsuperscript{-5} − P\textsubscript{L}; 8.71 × 10\textsuperscript{-2} − P\textsubscript{L} (estimated for heptachloronaphtalenes, Kaupp & McLachlan 1999)
Henry’s Law Constant (Pa·m\textsuperscript{3}/mol):
Octanol/Water Partition Coefficient, log K\textsubscript{ow} at 25°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-k’ correlation, HPLC-k’ correlation, Lei et al. 2000)
- log K\textsubscript{ow} = 2.998 + 1660.82/(T/K), temp range 5–55°C (temperature dependence HPLC-k’ correlation, Lei et al. 2000)
- 7.70 (GC-RT correlation, Hackenberg et al. 2003)
Octanol/Air Partition Coefficient, log $K_{OA}$ at 25°C or as indicated and the reported temperature dependence equations:

$$ \log K_{OA} = 10600/(2.303\cdot RT) - 7.20; \text{ temp range 10–50°C (GC-RT correlation, Su et al. 2002)} $$

**Bioconcentration Factor, log BCF or log $K_B$:**

- 2.50 ($Oncorhynchus mykiss$, Oliver & Niimi 1985; quoted, Crookes & Howe 1993)
- 2.52 (rainbow trout, mean value, Oliver & Niimi 1985)
- 5.0 (calculated-$K_{OW}$ and $S_0$, Banerjee & Baughman 1991)
- 2.52 ($Oncorhynchus mykiss$, under flow-through condition, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log $K_{OC}$:

- 5.38 (estimated, Crookes & Howe 1993)

**Environmental Fate Rate Constants, $k$ and Half-Lives, $t_{1/2}$:**

- **Volatilization:**
- **Photolysis:**

$$ t_{1/2} = 1608–16082 \text{ h based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).} $$

- **Hydrolysis:**

$$ t_{1/2} = 1608–16082 \text{ h based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).} $$

- **Biodegradation:**

- Aerobic biodegradation $k_2 = 4320–8760$ h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991);
- Anaerobic biodegradation $t_{1/2} = 17280–35040$ 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 ($k_1$ and $k_2$):

**Half-Lives in the Environment:**

- **Air:**

$$ t_{1/2} = 1608–16082 \text{ h in air based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).} $$

- **Surface water:** $t_{1/2} = 1608–16082 \text{ h based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).} $$

- **Ground water:** $t_{1/2} = 8640–17520$ h, based on essentially no biodegradation observed for hexachloro-benzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).

- **Sediment:**

$$ t_{1/2} = 4320–8760 \text{ h, based on essentially no biodegradation observed for hexachlorobenzene in soil die-away tests (Griffin & Chou 1981; quoted, Howard et al. 1991).} $$

- **Biota:**
**4.1.4 BROMINATED POLYNUCLEAR AROMATIC HYDROCARBONS**

### 4.1.4.1 1-Bromonaphthalene

![Chemical Structure of 1-Bromonaphthalene]

**Common Name:** 1-Bromonaphthalene  
**Synonym:** α-bromonaphthalene  
**Chemical Name:** 1-bromonaphthalene  
**CAS Registry No:** 90-11-9  
**Molecular Formula:** C\textsubscript{10}H\textsubscript{7}Br  
**Molecular Weight:** 207.067  
**Melting Point (°C):** 6.1 (Lide 2003)  
**Boiling Point (°C):** 281 (Lide 2003)  
**Density (g/cm\textsuperscript{3} at 20°C):** 1.4834 (Dean 1992)  
**Molar Volume (cm\textsuperscript{3}/mol):** 140.6 (30°C, calculated from density, Stephenson & Malanowski 1987)  
**Dissociation Constant pK\textsubscript{a}:**  
**Enthalpy of Vaporization, ∆H\textsubscript{v} (kJ/mol):** 39.33 (at normal bp, Hon et al. 1976)  
**Enthalpy of Fusion, ∆H\textsubscript{fus} (kJ/mol):**  
**Entropy of Fusion, ∆S\textsubscript{fus} (J/mol K):**  
**Fugacity Ratio at 25°C, F:** 1.0  
**Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C):** 9.95 (Yalkowsky et al. 1983)  
**Vapor Pressure (Pa at 25°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* (97.9°C, static-Hg manometer, measured range 97.9–281.1°C, Kahlbaum 1898)  
133* (84.2°C, summary of literature data, temp range 84.2–281.1°C, Stull 1947)  
log (P/mmHg) = (–0.2185 × 13274.9/(T/K)) + 8.131285; temp range 84.2–281.1°C, (Antoine eq., Weast 1972–73)  
196.27°C, ebulliometry, measured range 97.9–285.92°C, Hon et al. 1976)  
log (P/mmHg) = 5.38175 – 929.64/(91.06 + t/°C); temp range: 196.27–285.93°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 (P/kPa) = (6.90 – 2950/(T/K), temp range 295–359 K (torsion and Knudsen effusion, Urbani et al. 1980)  
log (P/mmHg) = 7.00350 – 1927.05/(186.0 + t°C); temp range: liquid (Antoine eq., Dean 1985, 1992)  
log (P\textsubscript{L}/kPa) = 6.56365 – 2303.73/[–48.841 + (T/K)]; temp range 357–555 K (liquid, Antoine eq.-I, Stephenson & Malanowski 1987)
log (P/kPa) = 4.50679 – 929.871/(182.045 + (T/K)), temp range 469–559 K, (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

2.754* (30.15°C, transpiration method, measured range 303.3–336.3 K, Verevkin 2003)

ln (P/Po) = 299.001/R – 8.3941.481/R·(T/K) – 73.5/R·ln[(T/K)/298.15], where Po = 101.325 kPa, gas constant R = 8.31451 J·K\(^{-1}\)·mol\(^{-1}\) (vapor pressure eq. from transpiration measurement, temp range 303.3–336.3 K, Verevkin 2003)

Henry’s Law Constant (Pa·m\(^3\)/mol):

Octanol/Water Partition Coefficient, log \(K_{\text{OW}}\):

4.35 (calculated-fragment const., Yalkowsky et al. 1983)

Octanol/Air Partition Coefficient, log \(K_{\text{OA}}\):

Bioconcentration Factor, log BCF or log \(K_{\text{B}}\):

Sorption Partition Coefficient, log \(K_{\text{OC}}\):

Environmental Fate Rate Constants, k or Half-Lives, \(t_{1/2}\):

Half-Lives in the Environment:

<table>
<thead>
<tr>
<th>TABLE 4.1.4.1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reported vapor pressures of 1-bromonaphthalene at various temperatures and the coefficients for the vapor pressure equations</td>
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<thead>
<tr>
<th></th>
<th>log P = A – B/(T/K)</th>
<th>ln P = A – B/(T/K)</th>
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<tbody>
<tr>
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<td>log P = A – B/(C + t/°C)</td>
<td>ln P = A – B/(C + t/°C)</td>
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<td></td>
<td>log P = A – B/(C + T/K)</td>
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<td>log P = A – B/(T/K) – C·log (T/K)</td>
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1. Kahlbaum 1898: static method-manometer

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<th>P/Pa</th>
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<td>266</td>
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<tr>
<td>157.2</td>
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<td>170.2</td>
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2. Stull 1947: summary of literature data

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<th>P/Pa</th>
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<tr>
<td>277.2</td>
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3. Hon et al. 1976: ebulliometry

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4. Urbani et al. 1980: torsion effusion

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<td>25</td>
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TABLE 4.1.4.1.1 (Continued)

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<td>ebulliometry</td>
<td>torsion effusion</td>
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<td></td>
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\[ \Delta H_v/(kJ \text{ mol}^{-1}) = 39.33 \]

at bp

2.

Urbani et al. 1980
(Continued)

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For Knudsen effusion:

\[ \Delta H_v/(kJ \text{ mol}^{-1}) = 63.91 \]

at 298.15 K

Overall temp dependence eq. 1

<table>
<thead>
<tr>
<th>P/kPa</th>
<th>[ R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} ]</th>
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<tr>
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<td>eq. 2</td>
<td>P/kPa</td>
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<td>eq. 4a</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>eq. 1</td>
<td>P/kPa</td>
</tr>
<tr>
<td>eq. 1</td>
<td>6.90 ± 1.1</td>
</tr>
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</table>

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FIGURE 4.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for 1-bromonaphthalene.
4.1.4.2 2-Bromonaphthalene

Common Name: 2-Bromonaphthalene
Synonym: β-bromonaphthalene
Chemical Name: 2-bromonaphthalene
CAS Registry No: 580-13-2
Molecular Formula: C_{10}H_{7}Br
Molecular Weight: 207.067
Melting Point (°C): 55.9 (Lide 2003)
Boiling Point (°C): 281.5 (Lide 2003)
Density (g/cm³ at 20°C): 1.463 (Ruelle & Kesselring 1997)
Molar Volume (cm³/mol): 170.9 (calculated-Le Bas method at normal boiling point)

Dissociation Constant $pK_a$:
Enthalpy of Fusion, $\Delta H_{\text{fus}}$ (kJ/mol): 11.97 (Ruelle & Kesselring 1997)
Entropy of Fusion, $\Delta S_{\text{fus}}$ (J/mol K):
Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K), F: 0.498 (mp at 55.9°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated): 8.27 (Yalkowsky et al. 1983)
7.72 (calculated-molecular connectivity indices, Nirmalakhandan & Speece 1989)
3.80, 8.04, 15.76 (4, 25, 40°C, 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)

Vapor Pressure (Pa at 25°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°C, solid I, transpiration method-GC, measured range 280.4–318.3 K, Verevkin 2003)
\[ \ln \left( \frac{P}{P_0} \right) = \frac{314.110}{R} - \frac{94001.596}{R \cdot (T/K)} - \left( \frac{41.6}{R} \right) \ln \left[ \frac{T}{298.15} \right], \text{ where } P_0 = 101.325 \text{ kPa, gas constant } R = 8.31451 \text{ J/K} \cdot \text{mol}^{-1} \text{ (solid I, vapor pressure eq. from transpiration measurement, temp range 280.4–318.3 K, Verevkin 2003)}
\]
7.34* (46.05°C, solid-II, transpiration method-GC, measured range 319.2–328.2 K, Verevkin 2003)
\[ \ln \left( \frac{P}{P_0} \right) = \frac{302.672}{R} - \frac{90417.272}{R \cdot (T/K)} - \left( \frac{41.6}{R} \right) \ln \left[ \frac{T}{298.15} \right], \text{ where } P_0 = 101.325 \text{ kPa, gas constant } R = 8.31451 \text{ J/K} \cdot \text{mol}^{-1} \text{ (solid II, vapor pressure eq. from transpiration measurements, temp range 319.2–328.2 K, Verevkin 2003)}
\]
18.75* (57.05°C, liquid, transpiration method-GC, measured range 330.2–360.2 K, Verevkin 2003)
\[ \ln \left( \frac{P}{P_0} \right) = \frac{303.761}{R} - \frac{89574.863}{R \cdot (T/K)} - \left( \frac{78.8}{R} \right) \ln \left[ \frac{T}{298.15} \right], \text{ where } P_0 = 101.325 \text{ kPa, gas constant } R = 8.31451 \text{ J/K} \cdot \text{mol}^{-1} \text{ (liquid, vapor pressure eq. from transpiration measurements, temp range 330.2–360.2 K, Verevkin 2003)}
\]

Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log $K_{\text{ow}}$:
4.35 (calculated-fragment const., Yalkowsky et al. 1983)
Octanol/Air Partition Coefficient, log $K_{OA}$:

Bioconcentration Factor, log BCF or log $K_B$:

Sorption Partition Coefficient, log $K_{OC}$:

Environmental Fate Rate Constants, $k$ or Half-Lives, $t_\text{½}$:

Half-Lives in the Environment:

### TABLE 4.1.4.2.1

Reported vapor pressures of 2-bromonaphthalene at various temperatures and the coefficients for the vapor pressure equations

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>solid I</th>
<th>solid II</th>
<th>solid II</th>
<th>liquid</th>
<th>P/Pa</th>
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<td>P/Pa</td>
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<tr>
<td>7.25</td>
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<td>66.15</td>
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<td>11.47</td>
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<td>eq. 4a</td>
<td>P/kPa</td>
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<td>P/kPa</td>
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<td>P/kPa</td>
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<td>eq. 4a</td>
<td>P/kPa</td>
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<td>P/kPa</td>
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</tr>
<tr>
<td>101.325 kPa</td>
<td>A 302.672/R</td>
<td>B 90417.272/R</td>
<td>C 41.6/R</td>
<td>R = 8.314 J K⁻¹ mol⁻¹</td>
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</tr>
<tr>
<td>314.110/R</td>
<td>B 90417.272/R</td>
<td>C 41.6/R</td>
<td>R = 8.314 J K⁻¹ mol⁻¹</td>
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<tr>
<td>94001.596/R</td>
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<td>R = 8.314 J K⁻¹ mol⁻¹</td>
<td></td>
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<tr>
<td>41.6/R</td>
<td>R = 8.314 J K⁻¹ mol⁻¹</td>
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<tr>
<td>eq. 4a</td>
<td>P/kPa</td>
<td>P/kPa</td>
<td>eq. 4a</td>
<td>P/kPa</td>
<td>P/kPa</td>
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<td>101.325 kPa</td>
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<td>R = 8.314 J K⁻¹ mol⁻¹</td>
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<tr>
<td>94001.596/R</td>
<td>C 41.6/R</td>
<td>R = 8.314 J K⁻¹ mol⁻¹</td>
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<tr>
<td>41.6/R</td>
<td>R = 8.314 J K⁻¹ mol⁻¹</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

$\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 81.60$ at 298.15 K

$\Delta H_{\text{subl}}/(kJ \text{ mol}^{-1}) = 78.01$ at 298.15 K

$\Delta H = 66.08$ at 298.15 K
FIGURE 4.1.4.2.1 Logarithm of vapor pressure versus reciprocal temperature for 2-bromonaphthalene.
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: C_{10}H_{6}Br_{2}
Molecular Weight: 285.963
Melting Point (°C):
  83  (Lide 2003)
Boiling Point (°C):
  310  (Lide 2003)
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
   194.2  (calculated-Le Bas method at normal boiling point)
Dissociation Constant pKₐ:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.27 (mp at 83°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated):
   0.125, 0.35, and 0.866 (4, 25, and 40°C, generator column-GC/ECD, Dickhut et al. 1994)
   1.92  (calculated-TSA, Dickhut et al. 1994)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{OW}:
Octanol/Air Partition Coefficient, log K_{OA}:
Bioconcentration Factor, log BCF or log K_{bi}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k or Half-Lives, t_{½}:
Half-Lives in the Environment:
4.1.4.4 2,3-Dibromonaphthalene

Common Name: 2,3-Dibromonaphthalene
Synonym:
Chemical Name: 2,3-dibromonaphthalene
CAS Registry No: 
Molecular Formula: C_{10}H_{6}Br_{2}
Molecular Weight: 285.963
Melting Point (°C):
  140  (Lide 2003)
Boiling Point (°C):
Density (g/cm^3 at 20°C):
Molar Volume (cm^3/mol):
  194.2  (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0744 (mp at 140°C)
Water Solubility (g/m^3 or mg/L at 25°C):
  0.0554, 0.138, and 0.352 (4, 25, and 40°C, generator column-GC/ECD, Dickhut et al. 1994)
  0.432  (calculated-TSA, Dickhut et al. 1994)
Vapor Pressure (Pa at 25°C):
Henry's Law Constant (Pa·m^3/mol):
Octanol/Water Partition Coefficient, log K_{ow}:
Octanol/Air Partition Coefficient, log K_{oa}:
Bioconcentration Factor, log BCF or log K_B:
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k or Half-Lives, t_{1/2}:
Half-Lives in the Environment:
4.1.4.5 4-Bromobiphenyl

Common Name: 4-Bromobiphenyl
Synonym:
Chemical Name: 4-bromobiphenyl
CAS Registry No: 92-66-0
Molecular Formula: C₁₂H₉Br
Molecular Weight: 233.103
Melting Point (°C):
91.5 (Lide 2003)
Boiling Point (°C):
310 (Weast 1983–84; Stephenson & Malanowski 1987, Lide 2003)
Density (g/cm³ at 25°C):
0.9327 (Weast 1983–84, Lide 2003)
Molar Volume (cm³/mol):
176.1 (Ruelle & Kesselring 1997)
207.9 (calculated-Le Bas method at normal boiling point)
Molar Volume (cm³/mol):
250.0 (25°C, calculated-density)
Dissociation Constant pKₐ:

Enthalpy of Fusion, ∆Hₘₖ (kJ/mol):
26.86 (Doucette & Andren 1988)
Entropy of Fusion, ∆Sₘₖ (J/mol K):

Fugacity Ratio at 25°C (assuming ∆Sₘₖ = 56 J/mol K), F: 0.223 (mp at 91.5°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations.):
0.235, 0.653, 0.874 (4.9, 25, 40°C, generator column-GC, Doucette & Andren 1988a)
S/(mol/L) = 9.36 × 10⁻⁷ exp(0.037t/°C) (generator column-GC/ECD, temp range 4.9–40°C, Doucette & Andren 1988a); or
log x = -1436/(T/K) – 1.541, temp range 4.9–40°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°C and reported temperature dependence equations):
log (Pₜ/kPa) = 2.24643 – 2174.97/(T/K) – 70.067; (Antoine eq., liquid state, temp range 371–583 K, Stephenson & Malanowski 1987)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kₗₗₗₗ:
4.96; 4.89, 5.00 (generator column-GC; calculated-group contribution method, estimated-TSA and Kₗₗₗₗ, Doucette & Andren 1987)
4.96; 4.89, 4.83, 5.10, 5.14, 5.10 (generator column-GC; calculated- const., HPLC-RT correlation, calculated-MW, calculated-MCI, calculated-TSA and Kₗₗₗₗ, Doucette & Andren 1988b)
4.96 (recommended, Sangster 1993)
4.95 (Hansch et al. 1995)
Octanol/Air Partition Coefficient, log Kₗₗₗₗ:
Bioconcentration Factor, log BCF or log Kₗₗₗₗ:
Sorption Partition Coefficient, log Kₗₗₗₗ:
Environmental Fate Rate Constants, k or Half-Lives, tₕₕ:
Half-Lives in the Environment:
4.1.4.6 4,4′-Dibromobiphenyl

Common Name: 4,4′-Dibromobiphenyl
Synonym: PBB-15, 4,4′-dibromo-1,1′-biphenyl
Chemical Name: 4,4′-dibromobiphenyl
CAS Registry No: 92-86-4
Molecular Formula: C\textsubscript{12}H\textsubscript{8}Br\textsubscript{2}
Molecular Weight: 312.000

Melting Point (°C):
164 (Ruelle & Kesselring 1997, Lide 2003)

Boiling Point (°C):
357.5 (Lide 2003)

Density (g/cm\textsuperscript{3}):
231.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, \(\Delta H_{\text{ fus}}\) (kJ/mol):

Entropy of Fusion, \(\Delta S_{\text{ fus}}\) (J/mol K):

Fugacity Ratio at 25°C (assuming \(\Delta S_{\text{ fus}} = 56\) J/mol K), F: 0.0433 (mp at 164°C)

Water Solubility (g/m\textsuperscript{3} or mg/L at 25°C or as indicated and reported temperature dependence equations):

Vapor Pressure (Pa at 25°C):

Henry’s Law Constant (Pa·m\textsuperscript{3}/mol):

Octanol/Water Partition Coefficient, log \(K_{\text{ ow}}\):

Octanol/Air Partition Coefficient, log \(K_{\text{ oa}}\):

Bioconcentration Factor, log \(K_{\text{ BF}}\) or log \(K_{\text{ B}}\):

Sorption Partition Coefficient, log \(K_{\text{ OC}}\):

Environmental Fate Rate Constants, k and Half-Lives, \(t_{\frac{1}{2}}\):

Bioconcentration and Uptake and Elimination Rate Constants (\(k_1\) and \(k_2\)):

Half-Lives in the Environment:
4.1.4.7 2,4,6-Tribromobiphenyl

![Chemical Structure](image)

**Common Name:** 2,4,6-Tribromobiphenyl  
**Synonym:** PBB-30  
**Chemical Name:** 2,4,6-tibromobiphenyl  
**CAS Registry No:** 59080-33-0  
**Molecular Formula:** C₁₂H₇Br₃  
**Molecular Weight:** 390.896  
**Melting Point (°C):** 64 (Ruelle & Kesselring 1997)  
**Boiling Point (°C):**  
**Density (g/cm³):**  
**Molar Volume (cm³/mol):**  
  - 208.3 (Ruelle & Kesselring 1997)  
  - 254.5 (calculated-Le Bas method at normal boiling point)  
**Enthalpy of Fusion, ΔHₙₑₑ (kJ/mol):**  
**Entropy of Fusion, ΔSₙₑₑ (J/mol K):**  
**Fugacity Ratio at 25°C (assuming ΔSₙₑₑ = 56 J/mol K), F:** 0.414 (mp at 64°C)  
**Water Solubility (g/m³ or mg/L at 25°C):**  
  - 0.016 (generator column-GC, Gobas et al. 1988)  
  - 0.0131 (quoted, Chessells et al. 1992)  
  - 0.054 (calculated-MCI χ, Ruelle & Kesselring 1997)  
**Vapor Pressure (Pa at 25°C):**  
**Henry’s Law Constant (Pa·m³/mol):**  
**Octanol/Water Partition Coefficient, log Kₚ₆₆:**  
  - 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 Kₐ₃:**  
**Bioconcentration Factor, log BCF or log K₉:**  
  - 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 χ, Kₚ₆₆, Lu et al. 1999)  
**Sorption Partition Coefficient, log K₀₆:**  
**Environmental Fate Rate Constants, k and Half-Lives, tₕ:**  
  - Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):  
    - log k₁ = 3.05 d⁻¹; log k₂ = −0.83 d⁻¹ (guppy, Gobas et al. 1989)  
  - Half-Lives in the Environment:
4.1.4.8 2,2',5,5'-Tetrabromobiphenyl

Common Name: 2,2',5,5'-Tetrabromobiphenyl
Synonym: PBB-52
Chemical Name: 2,2’,5,5’-tetrabromobiphenyl
CAS Registry No: 59080-37-4
Molecular Formula: C₁₂H₆Br₄
Molecular Weight: 469.792
Melting Point (°C): 144 (Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
Enthalpy of Fusion, ΔHfus (kJ/mol):
Entropy of Fusion, ΔSfus (J/mol K):
Fugacity Ratio at 25°C (assuming ΔSfus = 56 J/mol K), F: 0.068 (mp at 144°C)
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log Kow:
Bioconcentration Factor, log BCF or log Kb:
Sorption Partition Coefficient, log Koc:
Environmental Fate Rate Constants, k and Half-Lives, t½:
Bioconcentration and Uptake and Elimination Rate Constants (k₁ and k₂):
Half-Lives in the Environment:
4.1.4.9  2,2′,4,5,5′-Pentabromobiphenyl

Common Name: 2,2′,4,5,5′-Pentabromobiphenyl
Synonym:
Chemical Name: 2,2′,4,5,5′-pentabromobiphenyl
CAS Registry No: 6788-96-4
Molecular Formula: C_{12}H_{5}Br_{5}
Molecular Weight: 548.688
Melting Point (°C):
157  (Dickhut et al. 1994; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³ at 20°C):
Molar Volume (cm³/mol):
301.1  (calculated-Le Bas method at normal boiling point)
Dissociation Constant pK_a:
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
45.44  (Doucette & Andren 1988)
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.0507 (mp at 157°C)
Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations.):
1.032 × 10⁻⁴, 4.42 × 10⁻⁴, 9.82 × 10⁻⁴ (4.9, 25, 40°C, generator column-GC/ECD, Doucette & Andren 1988a)
S/(mol/L) = 1.52 × 10⁻¹⁰ exp(0.063·t/°C) (generator column-GC, temp range 4–40°C, Doucette & Andren 1988a)
log x = −2374/(T/K) − 2.373, temp range 4–40°C (generator column-GC, Doucette & Andren 1988a)
Vapor Pressure (Pa at 25°C):
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{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 K_{OA}:
Bioconcentration Factor, log BCF or log K_{B}:
Sorption Partition Coefficient, log K_{OC}:
Environmental Fate Rate Constants, k or Half-Lives, t_1/2:
Half-Lives in the Environment:
4.1.4.10 2,2',4,4',6,6'-Hexabromobiphenyl

Chemical Name: 2,2',4,4',6,6'-hexabromobiphenyl
CAS Registry No: 59261-08-4
Molecular Formula: C_{12}H_{4}Br_{6}
Molecular Weight: 627.584
Melting Point (°C):
   176 (Gobas et al. 1988; Ruelle & Kesselring 1997)
Boiling Point (°C):
Density (g/cm³):
   256.6 (Ruelle & Kesselring 1997)
   324.4 (calculated-Le Bas method at normal boiling point)
Enthalpy of Fusion, ΔH_{fus} (kJ/mol):
Entropy of Fusion, ΔS_{fus} (J/mol K):
Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 0.033 (mp at 176°C)
Water Solubility (g/m³ or mg/L at 25°C):
   6.23 × 10^{-4} (generator column-GC, Gobas et al. 1988)
   0.0210 (lit. mean, Chessells et al. 1992)
   1.04 × 10^{-4} (calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)
Vapor Pressure (Pa at 25°C):
   8.033 × 10^{-6} (for hexabrominated biphenyl, GC-RT correlation, Watanabe & Tatsukawa 1989)
   4.52 × 10^{-10} (quoted, Pijnenburg et al. 1995)
Henry's Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log K_{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 K_{oa}:
Bioconcentration Factor, log BCF or log K_{bi}:
   5.85 (guppy, lipid weight-based, Gobas et al. 1989)
   4.26 (calculated-K_{ow}, Chessells et al. 1992)
Sorption Partition Coefficient, log K_{oc}:
Environmental Fate Rate Constants, k and Half-Lives, t_{1/2}:
   Bioconcentration and Uptake and Elimination Rate Constants (k_{1} and k_{2}):
      log k_{1} = 2.51 d^{-1}; log k_{2} = -2.15 d^{-1} (guppy, Gobas et al. 1989)
   Half-Lives in the Environment:
4.1.4.11 Decabromobiphenyl

Common Name: Decabromobiphenyl
Synonym: PBB-209
Chemical Name:
CAS Registry No: 13654-09-6
Molecular Formula: C₁₂Br₁₀
Molecular Weight: 943.168
Melting Point (°C):
Boiling Point (°C):
Density (g/cm³):
Molar Volume (cm³/mol):
417.6 (calculated-Le Bas method at normal boiling point)
Heat of Fusion, \( \Delta H_{\text{fus}} \) (kJ/mol):
Entropy of Fusion, \( \Delta S_{\text{fus}} \) (J/mol K):
Fugacity Ratio at 25°C (assuming \( \Delta S_{\text{fus}} = 56 \) J/mol K), F:
Water Solubility (g/m³ or mg/L at 25°C):
Vapor Pressure (Pa at 25°C):
\( > 1.33 \times 10^{-9} \) (GC-RT correlation, Watanabe & Tatsukawa 1989)
\( < 7.4 \times 10^{-4} \) (quoted, Pijnenburg et al. 1995)
Henry’s Law Constant (Pa·m³/mol):
Octanol/Water Partition Coefficient, log \( K_{\text{OW}} \):
8.58; 12.63; 9.36 (generator column-GC; calculated-group contribution method, estimated-TSA and \( K_{\text{OW}} \), 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 \( K_{\text{OW}} \), Doucette & Andren 1988b)
8.60 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)
Octanol/Air Partition Coefficient, log \( K_{\text{OA}} \):
Bioconcentration Factor, log BCF or log \( K_{\text{B}} \):
Sorption Partition Coefficient, log \( K_{\text{OC}} \):
Environmental Fate Rate Constants, k and Half-Lives, \( t_{\frac{1}{2}} \):
Half-Lives in the Environment:
### TABLE 4.2.1
Summary of physical properties of polynuclear aromatic hydrocarbons (PAHs)

<table>
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<th>Compound</th>
<th>CAS no.</th>
<th>Molecular formula</th>
<th>Molecular weight, MW g/mol</th>
<th>m.p., °C</th>
<th>b.p., °C</th>
<th>Fugacity ratio, F at 25°C*</th>
<th>Molar volume, V_m, cm³/mol</th>
<th>MW/ρ at 20°C</th>
<th>Le Bas</th>
</tr>
</thead>
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<td>Indan</td>
<td>496-11-7</td>
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Note:
- 3-MCA = 3-Methylcholanthrene
- 7,12-DMBA = 7,12-Dimethylbenzo[a]anthracene
- 9,10-DMBA = 9,10-Dimethylbenzo[a]anthracene
- * Assuming $\Delta S_{ fus } = 56$ J/mol K.
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<th>Solubility</th>
<th>Henry's law constant</th>
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<td>$P_1$/Pa</td>
<td>$S_0$(g/m$^3$)</td>
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**Abbreviations:**
- 3-MCA: 3-Methylcholanthrene
- 7,12-DMBA: 7,12-Dimethylbenz[a]anthracene
- 9,10-DMBA: 9,10-Dimethylbenz[a]anthracene

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TABLE 4.2.3
Suggested half-life classes of polynuclear aromatic hydrocarbons (PAHs) in various environment compartments at 25°C

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<th>Water</th>
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<td>2</td>
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</tr>
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<td>4</td>
<td>6</td>
<td>7</td>
</tr>
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where,

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<th>Range (hours)</th>
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<tr>
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<td>10–30</td>
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<tr>
<td>3</td>
<td>55 (~ 2 days)</td>
<td>30–100</td>
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<tr>
<td>4</td>
<td>170 (~ 1 week)</td>
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<tr>
<td>5</td>
<td>550 (~ 3 weeks)</td>
<td>300–1,000</td>
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<tr>
<td>6</td>
<td>1700 (~ 2 months)</td>
<td>1,000–3,000</td>
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<tr>
<td>7</td>
<td>5500 (~ 8 months)</td>
<td>3,000–10,000</td>
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<td>8</td>
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<tr>
<td>9</td>
<td>55000 (~ 6 years)</td>
<td>&gt; 30,000</td>
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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.
4.3 REFERENCES


Hansch, C., Leo, A. (1979) *Substituent Constants for Correlation Analysis in Chemistry and Biology*. Wiley, N.Y.


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Polynuclear Aromatic Hydrocarbons (PAHs) and Related Aromatic Hydrocarbons


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