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Compilation of data for priority organic pollutants for derivation of Soil Guideline Values

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Steve Killeen

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Executive summary

This report provides a summary of recommended physical-chemical data for organic chemicals to help risk assessors derive assessment criteria for a range of soil contaminants using the Contaminated Land Exposure Assessment (CLEA) framework and software.

The CLEA framework is a tool to assess the risks to health from exposure to contaminated soil by adults and children living, working and playing on different types of land. It is used by the Environment Agency to derive Soil Guideline Values (SGV), that is, generic assessment criteria used to protect human health from chronic exposure to chemicals in soil.

In order to estimate human exposure, the CLEA model must predict the fate and transport of chemicals within the soil system and into air, water and plants. The physical-chemical properties of a contaminant are critical to understanding and modelling its fate and transport behaviour. Chemical data should be selected on a chemical-by-chemical basis. Variability in these reported properties may have a significant effect on the predicted soil behaviour of a chemical and ultimately on the risk assessment.

This report covers sixty-six organic chemicals that were identified by the Soil Guideline Value Taskforce as being a priority for the derivation of SGV. These chemicals include chlorinated solvents, pesticides, chlorobenzenes, chlorophenols, chlorotoluenes, organometallic compounds, petroleum hydrocarbons, and polycyclic aromatic hydrocarbons.

The following physical-chemical properties have been reviewed and are listed for each chemical:

- air-water partition coefficient
- boiling point and critical point temperature
- diffusion coefficients in air and water
- enthalpy of vapourisation
- octanol-water partition coefficient
- organic carbon-water partition coefficient
- vapour pressure
- water solubility.

The recommended values, collated from review of the scientific literature or estimated using reliable property estimation methods, can be used directly in the CLEA software to derive assessment criteria in accordance with guidance in the CLEA Software Handbook. These recommended values will also be used by the Environment Agency in the derivation of SGV.

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1 Introduction

1.1 Background

The Contaminated Land Exposure Assessment (CLEA) model assesses the risks to human health from exposure to contaminated soil by adults and children living, working and playing on different types of land (Environment Agency 2008a and 2008b). It is used by the Environment Agency in the derivation of **Soil Guideline Values** (SGV). SGV are **generic assessment criteria** that may be used to simplify the assessment of risk to human health from chronic **exposure** to chemicals in soil (Environment Agency 2008a).

In order to estimate human exposure, the CLEA model predicts the fate and transport of chemicals within the soil system and into air, water and plants (Environment Agency 2008a). Fate and transport of a chemical is a collective term to describe a number of complex and highly variable processes including:

- persistence of a chemical in soil, water and air;
- partitioning of a chemical between different environmental media (for example, a chemical may be adsorbed to soil organic matter, dissolved in the pore water solution, or in the soil vapour phase);
- transport of a chemical from one place to another (for example, **diffusion** of a chemical through soil into indoor or outdoor air spaces).

1.1.1 Fate and transport models

The fate and transport of chemicals in the soil environment depends on many different physical, chemical and biological processes. Ideally, monitoring data would be available to assess many of these processes for a wide range of chemicals (ECB 2003). However, this is seldom the case and chemical concentrations must be modelled.

Although more than a century of research has established the principles of how chemicals behave in the environment, predictive models are still in the early stages of development and appraisal. Many of these models are useful under the conditions for which they have been validated, although outside these boundaries their utility is limited and their reliability questionable (ECB 2003).

In general terms, two types of fate and transport model can be identified: (a) empirical and knowledge-based or (b) mathematical and mechanistic (ECB 2003). **Empirical models** are based on experimental observation and often establish plausible relationships between system parameters based on expert opinion. **Mechanistic models** establish plausible relationships based on scientific opinion but they are often more systematic and interpret the processes in the system from theoretical principles.

Empirical and mechanistic models range in complexity and the required number of input parameters (Environment Agency 2006, IPCS 2005). In undertaking both generic and detailed risk assessments, the choice of suitable model is based on its ability to accurately represent the conceptual model of the system being investigated, extent of validation and critical review, and the availability of good quality data to feed into the model for a range of circumstances.

The CLEA model uses several empirical and mechanistic models to provide a simplified understanding of fate and transport processes. The approach adopted is considered suitable for **generic quantitative risk assessment** and balances low data requirements with suitability for a wide range of chemicals and site conditions. It is consistent with good international practice. Fate and transport estimates depend on several parameter data sets including the physical-chemical properties of the soil contaminant and site conditions including soil type, wind conditions, and the physical dimensions of any buildings.

1.1.2 Physical and chemical data

The physical and chemical properties of a contaminant are critical to understanding and modelling its fate and transport in the environment. Chemical data should be selected on a chemical-by-chemical basis. For some properties, such as molecular weight, there will be very little variation in measurements reported in the scientific literature (Environment Agency 2003). However other properties, such as the octanol-water partition coefficient, may be subject to considerable variation due to differences in the experimental method or conditions used to measure its value or in the calculation used to derive the estimate from other **thermodynamic properties** (ECB 2003).[1] This variability in parameter may have a significant effect on the predicted contaminant behaviour and ultimately on the estimated human exposure.

In deriving assessment criteria, it is therefore important to adopt authoritative values for chemical data from reviews of the scientific and technical literature (Environment Agency 2003). All parameter choices should be fully justified and any description should include the sources examined, the range of values found, and where relevant, the temperature, pressure and other relevant conditions under which experimental data were defined. Whether the value has been measured experimentally or predicted using a **Quantitative Structure Activity Relationship** (QSAR) method should also be noted.[2] In many cases, chemical data for a single compound will be found across a number of different references. Care should be taken to ensure that related values for a single compound are consistent; for example, methods and experimental conditions used to measure **Henry's law constant** directly may be different from aqueous solubility and vapour pressure measurements (which can also be used to estimate the dimensionless form of Henry's law constant).

1.2 Methodology and report overview

This report is a review and summary of recommended physical-chemical data for the list of priority organic chemicals for the derivation of Soil Guideline Values. The methodology of the review is consistent with the principles described in the CLEA Report (Environment Agency 2008a) and the recommended values can be used directly in the CLEA software to derive generic and **site-specific assessment criteria** in accordance with guidance in the CLEA Software Handbook (Environment Agency 2008b). The review includes most priority organic chemicals in the CLEA Work Programme (see 1.2.1 for further information) and its recommendations supersede the

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[1] Another important source of experimental variability is the chemical itself, which may be obtained from a variety of different sources at varying degrees of purity.

[2] It is important when considering data estimated by a QSAR method that the chemical falls within the applicable range of the method (OECD 2007).

findings of Environment Agency Draft Technical Report P5-079/TR1 (Environment Agency 2003).

1.2.1 Priority organic chemicals

The report, *Potential Contaminants for the Assessment of Land (withdrawn publication)*, identified the priority chemicals for the development of Soil Guideline Values based on their likely presence in sufficient concentrations on many industrially affected UK sites to pose a risk to humans, buildings, water resources or ecosystems (Defra and Environment Agency 2002). In 2005, the Environment Agency asked members of the Soil Guideline Value Taskforce to review the priority chemicals for risks to human health in the context of producing new SGV reports to supplement those already published. After collating and analysing the responses received from members of the taskforce, the Environment Agency revised the list of priority chemicals as shown in Table 1.1. This priority list was used as the basis for selecting the organic chemicals reviewed in this report. [3]

Table 1.1 Updated priority chemicals list

Priority chemicals list for derivation of Soil Guideline Values[1]

Chemicals reviewed in this report are highlighted in bold[3]

acetone, **aldrin**, arsenic, asbestos, **atrazine**, **azinphos-methyl**, **benzene**, **benzo[a]pyrene**, beryllium, cadmium, chromium, **carbon disulphide**, **carbon tetrachloride**, **chloroform**, **chlorobenzenes**, **chlorophenols**, **chlorotoluenes**, copper, cyanide, **1,2-dichloroethane**, **dichlorvos**, **DDT**, **dieldrin**, dioxins and furans[2], **endosulfan**, **ethylbenzene**, explosives[2], **fenitrothion**, **hexachlorobuta-1,3-diene**, **hexachlorocyclohexanes**, lead, **malathion**, mercury, molybdenum, **naphthalene**, nickel, **organolead compounds**, **organotin compounds**, **pentachlorophenol**, **phenol**, **polychlorinated biphenyls**, **polycyclic aromatic hydrocarbons**, selenium, sulphur, **tetrachloroethane**, **tetrachloroethene**, thallium, **toluene**, total petroleum hydrocarbons[2], **1,1,1-trichloroethane**, **trichloroethene**, **trifluralin**, vanadium, **vinyl chloride**, **xylenes**, zinc

[1] Original nomenclature from *Potential Contaminants for the Assessment of Land* was used in this table

[2] Organic chemical group not included in this report (see sub-section 1.2.2)

[3] Inorganic chemicals are not included in this report. Data for inorganic chemicals will be provided in individual Soil Guideline Value reports.

1.2.2 Review methodology

What this report includes and what it does not

This report reviews and collates the physical-chemical data for 66 organic substances (including isomers) on the priority chemicals list (see 1.2.1). Where necessary, individual substances have been selected as representative of wide-ranging chemical groups as shown in Table 1.2, based on data availability and likely prevalence in soils. This should not be interpreted to mean that other chemicals within the group are not important in considering risks to health from soil contamination. The organic chemical groups not covered by this report are dioxins, explosives, polychlorinated biphenyls (PCBs), and total petroleum hydrocarbons, for the following reasons:

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[3] Several of the priority chemicals identified by the Soil Guideline Value Taskforce, are broad groups or families of chemicals (Defra and Environment Agency 2002). The chemicals included in this report are representative of these groups and were selected by the likely availability of physical-chemical and toxicity data in the scientific literature and their likely prevalence in the soil environment.

- Data for explosives has already been published (Environment Agency 2002).
- Data for dioxins and polychlorinated biphenyls will be based primarily on a review of data published by the University of Lancaster (Centre for Chemicals Management 2007).
- Data for total petroleum hydrocarbons relies on averaged information for hundreds of compounds and has already been comprehensively reviewed by the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG 1997).

Table 1.2 Representative chemical compounds and priority list groupings

Priority list group	Representative chemical compounds reviewed
Chlorobenzenes	chlorobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, 1,4-dichlorobenzene, hexachlorobenzene, pentachlorobenzene, 1,2,3,4-tetrachlorobenzene, 1,2,3,5-tetrachlorobenzene, 1,2,4,5-tetrachlorobenzene, 1,2,3-trichlorobenzene, 1,2,4-trichlorobenzene, 1,3,5-trichlorobenzene
Chlorophenols	2-chlorophenol, 2,4-dichlorophenol, 2,3,4,6-tetrachlorophenol, 2,4,6-trichlorophenol
Chlorotoluenes	α-chlorotoluene, 2-chlorotoluene, α,α,α-trichlorotoluene
Organolead compounds	tetraethyl lead
Organotin compounds	tributyl tin oxide
Polycyclic aromatic hydrocarbons	benz[a]anthracene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[ghi]perylene, benzo[a]pyrene, chrysene, dibenz[ah]anthracene, fluoranthene, indeno[123-cd]pyrene, naphthalene, pyrene

The physical-chemical data reviewed in this report are described in Chapter 2. This covers most but not all of the parameters needed by the CLEA model to derive Soil Guideline Values (Environment Agency 2008a and 2008b). The exceptions are:

- Toxicological information, which is outside the scope of this report and is discussed within the TOX guidance report (Environment Agency 2008c).
- Data on **dermal** absorption and plant uptake are rarely collated in the literature and for many priority organic chemicals there is very little primary research. Environment Agency (2008a) discusses default approaches for assessing these pathways in the absence of chemical data.

Review methodology

This review collated information from six authoritative desk references and three online databases as listed in Table 1.3. These resources are readily accessible and widely referenced by researchers and professionals in the UK and internationally.

Each reference was checked for data for each chemical, including typical synonyms, and the values recorded in a Microsoft ® Excel spreadsheet. Where a reference reported a range of values, the average at a specified temperature was calculated for all parameters with the exception of Henry's law constant, vapour pressure and water solubility where the geometric mean was reported. The geometric mean was preferred for values that typically varied by several orders of magnitude. Chemical data was corrected to consistent units according to the guidelines described in Chapter 2 and the temperature noted where different from 25°C. The collated data for nine different chemical properties is tabulated in Appendix A and is discussed further in Chapter 2.

Table 1.3 Information sources consulted for this review

Reference
HOWARD, P.H., 1990. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals* (3 Volumes). Chelsea: Lewis Publishers.
IUPAC-NIST, 2006. IUPAC-NIST Solubility Database, Version 1.0. NIST Standard Reference Database 106 (Updated 2006) [online]. Available from: http://srdata.nist.gov/solubility/index.asp
LIDE, D.R., 2008. *CRC Handbook of Chemistry and Physics*. Eighty-eigth Edition. Boca Raton, Florida: CRC Press.
MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. *Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*. Second Edition. Boca Raton: CRC Taylor & Francis.
MERCK, 2006. *The MERCK Index: An Encyclopedia of Chemicals, Drugs, and Biologicals*. Fourteenth Edition. (Editors) O'NEIL, M.J., HECKELMAN, P.E., KOCH, C.B., ROMAN, K.J., KENNY, C.M., D'ARECCA, M.R. Whitehouse Station, New Jersey: MERCK & Co., Inc.
MONTGOMERY, J.H., 2007. *Groundwater Chemicals Desk Reference*. Fourth Edition. Boca Raton, Florida: CRC Press.
MONTGOMERY, J.H., 1997. *Agrochemicals Desk Reference*. Second Edition. Boca Raton, Florida: CRC Press.
NIST, 2005. NIST Chemistry Web Book, NIST Standard Reference Database Number 69, June 2005 Release [online]. Available from: http://webbook.nist.gov/chemistry [accessed October 2007].
OECD, 2000. OECD Integrated HPV Database [online]. Available from: http://cs3-hq.oecd.org/scripts/hpv/ [accessed October 2008].

All references were given a broadly equal weighting for determining the recommended value, with a slight bias towards newer references when all other factors were tied. Each recommended value was also given a consensus rating to indicate the degree to which similar values were reported across all the references reviewed.

A low consensus rating indicated that the recommended value was found in only one or two references or that the degree of spread between values[4] was greater than five per cent. A high rating indicated that the recommended value was found in six or more references and the degree of spread around the central value was less than five per cent. This is a reasonably objective indicator of the spread of values for this chemical parameter in the literature reviewed from which the recommended value was selected. A high consensus value does not mean that the value is more likely to be correct or that there is a greater number of underlying studies upon which the reported data is based. The selection process is summarised in Table 1.4.

Where chemical data was unavailable in the literature, property estimation methods were employed. These methods were chosen based on recommendations made by EU (2003), Lyman *et al*. (1990), and Boethling and Mackay (2000), which are highly respected expert compilations, used throughout the world. Where multiple methods were available, consideration was given to ease of use and range of applicability as well as to accuracy. In most cases the accuracy of each estimation method was

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[4] These values are either (a) the value recommended by the individual source or (b) the mean, or geometric mean, of values from an individual source where no recommended value has been reported but one or more studies were reported.

checked against the available literature data to evaluate overall performance for the priority organic chemicals listed and to identify areas of high uncertainty. These methods are described in detail in Chapter 2.

Table 1.4 Selection process for recommended values and consensus values

Selection process [1, 2]	Consistency
▪ If all values the same, select this value. ▪ Select value from consistent range (if all values within the range are the same). ▪ Central value from consistent range (if all values in range are not the same). ▪ Newest value (if there is no consistent range or no single central value). ▪ In all cases, check reasonableness against underlying data.	▪ Very high (six or more references have same value) ▪ High (five references have same value or range covers six or more references) ▪ Medium (range covers four or five refs). ▪ Low (range covers two or three refs). ▪ Very low (no consistent range).

[1] Consistent range is defined as the range around a central tendency value of +/- five per cent for two or more references.

[2] All values typically reported at either 20 or 25°C. For water solubility, values at 10°C are identified separately, as temperature adjustment for this parameter cannot easily be predicted (see 2.10.3).

1.2.3 Report structure

The report consists of the following chapters:

Chapter 1	Introduces background to the report and the data collation / review process
Chapter 2	Describes the physical-chemical properties including unit conversions, temperature adjustments and property estimation methods
Chapter 3	A to Z summarises of the recommended physical-chemical data by contaminant
Appendices	Tabulated summary from review of authoritative sources and compiled data from use of estimation methods described in Chapter 2

2 Chemical properties

This chapter provides an introduction to the physical-chemical properties of contaminants including definition and use, data availability and variability, common unit conversions, adjustments for temperature dependence, and property estimation methods. This data is used in the CLEA software to predict the fate and transport of chemicals (Environment Agency 2008a and 2008b) or to estimate chemical properties using the methods described in this chapter.

The chemical properties are described in alphabetical order from air-water partition coefficient to water solubility and are listed in Table 2.1.

Table 2.1 Physical-chemical properties described in this chapter

Physical-chemical properties
Air-water partition coefficient (dimensionless) †
Boiling point at ambient pressure (K)
Critical point temperature at ambient pressure (K)
Diffusion coefficient in air (m^2 s^{-1})
Diffusion coefficient in water (m^2 s^{-1})
Enthalpy of vapourisation (kJ mol^{-1})
Octanol-water partition coefficient (dimensionless)
Organic carbon-water partition coefficient (cm^3 g^{-1})
Vapour pressure (Pa)
Water solubility (mg L^{-1})

Note

† Also known as the dimensionless form of the Henry's Law constant

2.1 Air-water partition coefficient

2.1.1 Definition and use

The air-water partition coefficient (K_{aw}) is the **constant of proportionality** between the concentration of a chemical in air and its concentration in water at low **partial pressures** and below its saturation limits in either air or water (Environment Agency 2008a). It can be estimated from **Henry's law constant** and is sometimes referred to as the dimensionless form of Henry's law constant.

William Henry studied the solubility of a gas in water as a function of pressure in 1803 (Boethling and Mackay 2000). Henry observed that a graphical plot of the concentration of a chemical in water expressed as a mole fraction x, versus the partial pressure of the chemical in the gaseous phase P, was typically linear at low partial pressures for many chemicals. This linearity was expressed as Henry's law, the constant of proportionality being Henry's law constant (H). It is calculated using Equation 2-1 (Boethling and Mackay 2000).

Equation 2-1

$$P = H \times C_w$$

P	Partial pressure of the chemical in the gaseous phase, Pa
H	Henry's law constant, Pa m^3 mol^{-1}
C_w	Concentration of the chemical in water, mol m^{-3}

Most environmental modellers would rather work with the chemical concentration in air than its partial pressure. Therefore, using the **ideal gas law**, the partial pressure of the chemical, *P*, in Equation 2-1 can be substituted by the concentration of the chemical in air (C_a) at a specified temperature to give Equation 2-2 (Boethling and Mackay 2000). In this equation, the temperature dependent Henry's law constant (*H/RT*) can be replaced by K_{aw}. A graphical plot of air concentration against water concentration will have a linear slope equal to K_{aw} until either phase reaches saturation point (Boethling and Mackay 2000).

Equation 2-2

$$C_a = \frac{H}{RT} C_w$$

C_a	Concentration of a chemical in air, mol m^{-3}
H	Henry's law constant, Pa m^3 mol^{-1}
R	Molar gas constant, Pa m^3 mol^{-1} K^{-1} [= 8.314472]
T	System temperature, K
C_w	Concentration of the chemical in water, mol m^{-3}

Along with the octanol-water partition coefficient (see 2.7),[5] K_{aw} determines how a chemical substance will partition between the three primary environmental media: air, water, and the organic matter present in soil and living things (Boethling and Mackay 2000). K_{aw} is used by the CLEA software to predict the partitioning of an organic contaminant between soil pore water and soil gas (Environment Agency 2008a).

2.1.2 Data availability and variability

Henry's law constant data for organic chemicals is widely available in the scientific literature, although there can be considerable variation in the values reported (see Table A4 in Appendix A). For example, the range of values observed for carbon disulphide in the literature review were between 142 Pa m^3 mol^{-1} at 20°C and 2,460,000 Pa m^3 mol^{-1} at 24°C (Howard 1990; Montgomery 2007). Henry's law constants are reported at a specified pressure (usually ambient) and temperature.

The methods for calculating K_{aw} in this chapter use Henry's law constant in units of Pa m^3 mol^{-1}. Common unit conversions are presented in Table 2.2.

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[5] In the absence of environmental partitioning data for many organic chemicals, the octanol-water partition coefficient is an important surrogate chemical property for describing fate and transport behaviour (see 2.7).

Table 2.2 Common unit conversions for Henry's law constant (NIST, 1995; Sander 1999)

Converting from	To Pascal per cubic metre per mole (Pa m^3 mol^{-1})
atm m^3 mol^{-1}	Multiply by 101,325
kPa m^3 mol^{-1}	Multiply by 1,000
mol kg^{-1} bar^{-1}	Divide by 100,000 to give mol kg^{-1} Pa^{-1}, multiply by 997 for values reported at 25°C (for values reported at 10°C multiply by 999.8) to give mol m^{-3} Pa^{-1}, and take reciprocal

2.1.3 Adjustments for temperature

K_{aw} and Henry's law constant vary with pressure and temperature because of their underlying dependence on chemical solubility in water and vapour pressure. Most data has been determined experimentally at ambient air pressure and therefore it is normally adjusted only for differences in temperature. In the CLEA software, K_{aw} should be determined at 10°C which is the assumed annual average temperature of UK surface soils (Environment Agency 2008a).

The US Environmental Protection Agency (USEPA 2001) provides a method for calculating K_{aw} at ambient temperature from Henry's law constant (H) for a chemical at a reference temperature (T_{ref}) using the Clapeyron equation. Most experimental values for H are reported in the literature at 20 or 25°C. This method requires that the boiling point (see 2.2), critical point temperature (see 2.3), and enthalpy of vaporisation (see 2.6) of the chemical are also known. Firstly, calculate the enthalpy of vaporisation (ΔH_{vap}) at the ambient soil temperature (Equation 2-3) using the values of exponent *n* in Table 2.3. Secondly, calculate K_{aw} using Equation 2-4.

Equation 2-3

$$\Delta H_{vap} = \Delta H_b \left[\frac{(1 - T_{amb} / T_c)}{(1 - T_b / T_c)} \right]^n$$

ΔH_{vap}	Enthalpy of vaporisation at the ambient soil temperature, J mol^{-1}
ΔH_b	Enthalpy of vaporisation at the normal boiling point, J mol^{-1}
T_{amb}	Ambient soil temperature, K [=283.15]
T_b	Chemical boiling point, K
T_c	Chemical critical point temperature, K
n	Empirical proportionality constant found from Table 2.3

Table 2.3 Values of exponent *n* as a function of boiling point (T_b) and critical point temperature (T_c)

T_B / T_C	Exponent *n*
< 0.57	0.30
0.57 – 0.71	0.74 (T_B / T_C) – 0.116
> 0.71	0.41

Equation 2-4

$$K_{aw} = \frac{EXP\left[-\frac{\Delta H_{vap}}{R}\left(\frac{1}{T_{amb}} - \frac{1}{T_{ref}}\right)\right]H}{RT_{amb}}$$

K_{aw}	Air-water partition coefficient at ambient soil temperature, dimensionless
H	Henry's law constant at the reference temperature, Pa m^3 mol^{-1}
ΔH_{vap}	Enthalpy of vaporisation at the ambient soil temperature, J mol^{-1}
T_{amb}	Ambient soil temperature, K [=283.15]
T_{ref}	Reference temperature for the Henry's law constant (H), K
R	Molar gas constant, in J mol^{-1} K^{-1} or Pa m^3 mol^{-1} K^{-1} [= 8.314472]

2.1.4 Methods for estimation

There are two recommended methods for estimating K_{aw} at the correction temperature. Boethling and Mackay (2000) noted that the simplest approach is to estimate K_{aw} by experimental measurement using either its concentration in air and water at the correct temperature and pressure (see Equation 2-5) or from its saturated vapour pressure and water concentration (see Equation 2-6). The latter is applicable to organic chemicals with a solubility of only a few per cent in water and the vapour pressure and water solubility data must also be from the same physical state, either solid or liquid depending on melting point. However, such data is rarely available in the literature at 10°C.

Equation 2-5

$$K_{aw} = \frac{C_a}{C_w}$$

K_{aw}	Air-water partition coefficient at ambient soil temperature, dimensionless
C_a	Concentration of a chemical in air at 10°C, mol m^{-3}
C_w	Concentration of the chemical in water at 10°C, mol m^{-3}

Equation 2-6

$$K_{aw} = \frac{P}{C_W RT_{amb}}$$

K_{aw}	Air-water partition coefficient at ambient soil temperature, dimensionless
P	Saturated vapour pressure of the pure chemical at 10°C, Pa
C_w	Saturated concentration of the chemical in water at 10°C, mol m^{-3}
R	Molar gas constant, Pa m^3 mol^{-1} K^{-1} [= 8.314472]
T_{amb}	Ambient soil temperature, K [=283.15]

Note that the Henry's law constant, H, is the ratio of P over C_w

Table B1 in Appendix B provides calculated K_{aw} values for 21 substances from the priority chemicals list. As noted in 2.9.4, vapour pressure may be estimated at 10°C and therefore this method is only limited by the availability of water solubility data. Methods for estimating water solubility are discussed in 2.10.4 but relate to 25°C.

In the absence of solubility data, K_{aw} may still be estimated at 10°C by using the Clapeyron relationship described in 2.1.3, provided that Henry's law constant is known at a reference temperature (usually 25°C). In the absence of a measured or literature value for H at 25°C, it can be estimated from the ratio of saturated vapour pressure to water solubility (based on Equation 2-6) or by using the structural contribution method proposed by Hine and Mookerjee (1975) and updated by Meylan and Howard (1991). Hine and Mookerjee (1975) related the **hydrophilic** character of a substance to its molecular structure using an empirical correlation of data on the free energy of transfer of organic compounds from the gas phase to aqueous solution of 345 chemicals. They developed two additive contribution schemes, one based on bond fragments (such as C-Cl or C=C) and the other using **functional groups** (such as CH_3 or OH). USEPA (2008) noted that the group contribution method is usually preferred but that its applicability is more limited because many of the group fragments have not yet been defined. Boethling and Mackay (2000) concluded that the Meylan and Howard method was a generally better method for estimating the Henry's law constant of hydrocarbons, halogenated hydrocarbons, esters, alcohols and phenols than more complex methods based on molecular connectivity/polarizability.

Table B2 in Appendix B compares the direct calculation (see Equation 2-6) and Meylan and Howard (1991) estimation methods with the recommended literature data for the priority organic chemicals. HENRYWIN Version 3.1 was used to implement the Meylan and Howard method, which is a computer program published by USEPA. It is available to download for free as part of the EPI software suite for most Windows-based PCs (USEPA 2008). HENRYWIN requires the molecular structure to be entered in SMILES notation and this information was obtained for the priority chemicals by downloading the relevant 2D MOL files from the NIST Webbook (NIST 2005). Although the group contribution method by Meylan and Howard (1991) was generally as accurate as the direct calculation method, it was applicable to about a third fewer chemicals. While the average absolute error for both approaches was around 15 per cent, there was a significant number of substances with errors of an order of magnitude or higher. Overall, the direct calculation method for determining Henry's Law constant is preferred if experimental or estimated data on vapour pressure and water solubility are available.

Table B3 in Appendix B summarises the K_{aw} values at 10°C for the priority chemicals by using the Clapeyron relationship (see 2.1.3). In most cases, the recommended literature value for the Henry's law constant at 20 or 25°C was used in the calculation. These values are recommended for use in the CLEA software for the derivation of Soil Guideline Values.

2.2 Boiling point

2.2.1 Definition and use

The boiling point of a chemical is defined as "*the temperature at which a liquid's vapour pressure equals the pressure of the atmosphere on the liquid*" (Boethling and Mackay 2000). If the pressure is exactly one atmosphere (that is, 101,325 Pa), the temperature is referred to as the *normal boiling point*. Pure chemicals have a unique boiling point and this is often used to identify compounds in laboratory investigations. Mixtures of two or more compounds have a boiling point range (Boethling and Mackay 2000).

The range of normal boiling points for organic chemicals is -162°C for methane to over 700°C for some polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs) and dioxins/furans. Many organic chemicals decompose at temperatures lower than their hypothetical boiling points, estimating this value for such thermally unstable compounds remains important because of its relationship with other chemical properties (Boethling and Mackay 2000).

Knowing the boiling point of an organic chemical is important for three reasons (Boethling and Mackay 2000):

- It defines the uppermost (theoretical) temperature at which a chemical can exist as a liquid.
- It serves as an indicator of chemical volatility, with higher boiling points associated with a lower volatility.
- It is a key parameter in the temperature adjustment of other physical -chemical data including the air-water partition coefficient and vapour pressure.

Boiling point depends on the strength of the intermolecular forces that hold molecules together (Brady and Holum 1993). Non-**polar chemicals** tend to be governed by weak intermolecular forces (known as ***van der Waals forces***), which increase gradually with increasing molecular weight (Brady and Holum 1993). Boethling and Mackay (2000) noted that for non-polar chemicals, boiling point correlates reasonably well with molecular weight. Polar chemicals tend to be governed by stronger intermolecular bonds resulting from **dipole-dipole attractions** and their resulting boiling points are much higher than would be predicted based on van der Waals forces only (Brady and Holum 1993). For example, if it were not for the **hydrogen bonding** between water molecules, water would have a boiling point around -80 °C.

2.2.2 Data availability and variability

Boiling point data for organic chemicals are widely available in the scientific literature with the notable exception of **pesticides** (see Table A1 in Appendix A). Many pesticides are known to decompose at temperatures lower than the normal boiling point and, if reported, the boiling point values are at much lower pressures than ambient conditions (Mackay *et al*. 2006, Montgomery 1997). There is often good agreement between authoritative sources on boiling point data, with variability often much less than one per cent.

The estimation and adjustment methods described in this report require the normal boiling point in units of Kelvin. Common unit conversions are presented in Table 2.4 (NIST 1995).

Table 2.4 Common unit conversions for normal boiling point (NIST 1995)

Converting from	To Kelvin (K)
degree Celsius (°C)	Add 273.15
degree Fahrenheit (°F)	Add 459.67, divide by 1.8

2.2.3 Adjustments for temperature

There are no temperature adjustments for this parameter.

2.2.4 Methods for estimation

Boethling and Mackay (2000) list more than twenty methods for estimating the normal boiling point of a chemical, which are primarily based on structural information about the molecule including molecular weight, bonds and functional groups, and symmetry. Many of these methods have been applied only to specific chemical classes such as alcohols and polycyclic aromatic hydrocarbons, and substituted benzenes.

No one method can provide simple and accurate estimates of boiling points across all chemical classes, although most methods have average absolute errors of 10-30°C or about two to five per cent (Boethling and Mackay 2000). Two generic methods are presented here, primarily for chemicals containing only carbon, hydrogen, oxygen, nitrogen or sulphur and the halogens. Several pesticides on the priority organic chemicals list also contain phosphorus and these were included. Method performance was evaluated by comparing predicted values with those recommended by the authoritative literature; the results are presented in Appendix C.

If the melting point of the chemical is known, the best performing of these methods is the Melting Point Correlation (Boethling and Mackay 2000, Walters *et al*. 1995) and this is recommended for the derivation of data for Soil Guideline Values. This method assumes that boiling point can be predicted from melting point by adjusting for the size and shape of the molecule and the extent of any hydrogen bonding. The empirical relationship is shown in Equation 2-7.

Equation 2-7

$$T_b = 181 + 0.510T_m - 47.6\log\sigma + 15.8Z + 12.5HB$$

T_b	Boiling point, K
T_m	Melting point, K
σ	Molecular symmetry number, unitless
Z	Modified count of the number of atoms in the molecule, unitless
HB	Number of donor hydrogen atoms in a hydrogen-bonding molecule, unitless

The molecular symmetry number, σ, is obtained by imagining all identical atoms to be labelled, and then counting the number of different but equivalent arrangements that can be obtained by rigidly rotating (but not reflecting) the molecule (Dannenfelser *et al*. 1993, McNaught and Wilkinson 1997). The modified count of the number of atoms, Z, is obtained by counting each type of atom and multiplying each total by the following coefficients: zero for hydrogen and fluorine, one for carbon, nitrogen, oxygen and chlorine, two for bromine and sulphur, and four for iodine. For example, aldrin has the chemical formula $C_{12}H_8Cl_6$, and a Z number of 18 (that is, 8*0 + 12*1 + 6*1). HB is the number of donor hydrogen atoms in alcohols, phenols, primary and secondary amines, carboxylic acids, and primary and secondary amides (Walters *et al*. 1995).

The empirical coefficients in Equation 2-7 were established for a test set of 1,419 chemicals including non-polar, polar, and hydrogen-bonded compounds (Walters *et al*. 1995). There was a strong linear correlation ($r^2 = 0.913$) and all variables were reported to be significant at the 95 per cent confidence level. Compared with measured data from 53 compounds on the priority organic chemicals list, this method had an average absolute error of four per cent (see Appendix C). An error of 27 per cent was observed for DDT, a chemical that was identified by Walters *et al*. (1995) as likely to give rise to large errors because of its "unstable nature".

The Banks' method uses a correlation with molecular weight and is shown in Equation 2-8 (Boethling and Mackay 2000). It is useful for estimating the boiling point of a compound with unusual elements, functional groups, and/or structural features.

Equation 2-8

$$\log T_b = 2.98 - \frac{4}{\sqrt{M}}$$

T_b	Boiling point, K
M	Molecular weight, g mol^{-1}

In a test with 70 compounds, Boethling and Mackay (2000) found that the Banks' method had an average absolute error of nine per cent. Compared with measured data from 55 compounds on the priority organic chemicals list, this method had an average absolute error of 12 per cent (see Appendix C). In particular, the Banks' method consistently underpredicted the boiling point of polycyclic aromatic hydrocarbons by a quarter to a third.

2.3 Critical point temperature

2.3.1 Definition and use

The critical point of a pure substance is the temperature and pressure at which the liquid and gas phases become indistinguishable and form a single dense fluid phase (see Figure 2-1). The critical point temperature, or the critical temperature (T_c), is the temperature measured or calculated at the critical point and is usually significantly above the ambient range (Boethling and Mackay 2000, USEPA 2001). For many organic substances, decomposition occurs below the critical point temperature.

The critical point temperature is used in environmental modelling to estimate the temperature dependence of the air-water partition coefficient and to adjust its value from reference to ambient conditions (see 2.1.3). Many of the factors which influence the boiling point also apply to the critical point temperature (see 2.2.1).

2.3.2 Data availability and variability

Critical point temperature data for organic chemicals are not widely available. In the authoritative references reviewed for this study, this parameter was reported for only 20 substances including benzene, carbon disulphide, simple chlorinated compounds, toluene and xylene. See Table A2 in Appendix A for a complete list of values obtained by the review for the priority organic chemicals identified in 1.2.1.

The calculations described in 2.1.3 require the critical point temperature in units of Kelvin. Common unit conversions are presented in Table 2.5 (NIST 1995).

Table 2.5 Common unit conversions for critical point temperature (NIST 1995)

Converting from	To Kelvin (K)
degree Celsius (°C)	Add 273.15
degree Fahrenheit (°F)	Add 459.67, divide by 1.8

2.3.3 Adjustments for temperature

There are no temperature adjustments for this parameter.

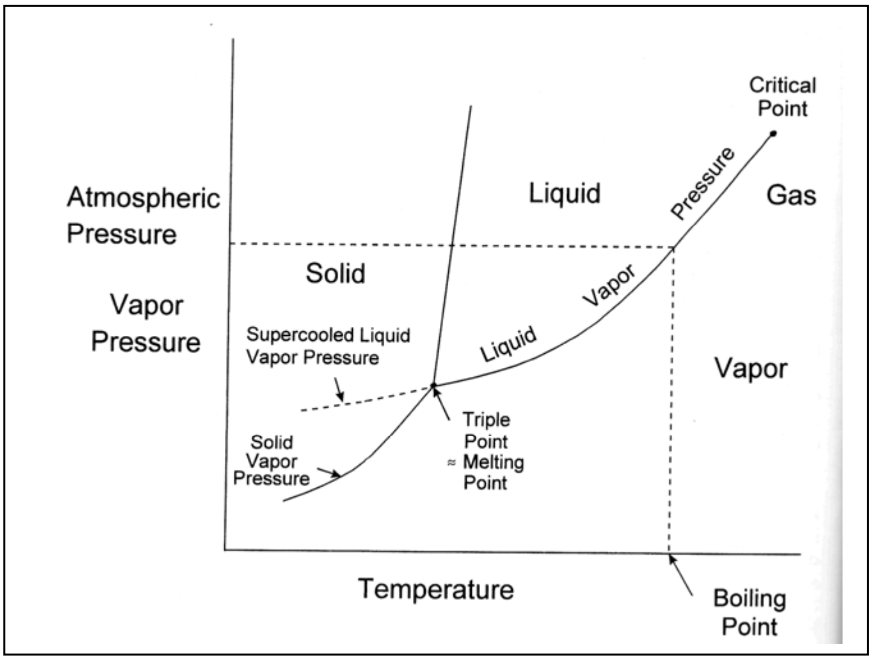

Figure 2-1: Diagram of phase relationships and reference markers including melting point, boiling point, and critical point (after Boethling and Mackay 2000). (Copyright © 2000 From *Handbook of Property Estimation Methods* by Boethling and Mackay. Reproduced by permission of Taylor and Francis Group, LLC, a division of Informa plc.)

2.3.4 Methods for estimation

There are two methods for estimating the value of critical point temperature for a pure substance (Lyman *et al.* 1990). Several chemists including Forman, Guldberg, and Thodos have reported that the ratio between boiling point and critical point temperature is relatively constant for many organic compounds and can be described by the relationship in Equation 2-9. For cases where the normal boiling point of a chemical is known, the critical point temperature can therefore be estimated.

Equation 2-9

$$T_b = \theta T_c$$

T_b	Boiling point, K
T_c	Critical point temperature, K
θ	Temperature ratio, dimensionless

Guldberg showed that for many organic chemicals, the temperature ratio (θ) was close to two-thirds and this is a useful approximation (Lyman *et al*. 1990, USEPA 2001). The ratio may be more accurately estimated using the Lydersen method shown in Equation 2-10 (Lyman *et al*. 1990). In this method, the temperature ratio is adjusted by accounting for different atomic and molecular features including functional groups and bonding types. Lyman *et al*. (1990) provides further detail on this method including a complete list of the functional groups and their incremental adjustment values.

Equation 2-10

$$\theta = 0.567 + \sum \Delta T - (\sum \Delta T)^2$$

θ	Temperature ratio, dimensionless
ΔT	Empirical factor based on the atomic and structural features of the molecule, dimensionless

In the absence of the normal boiling point, the critical point temperature can be estimated directly using the Forman-Thodos method (Lyman *et al*. 1990). However, it is unlikely that this method will be required for substances considered using the CLEA software because of the need to specify the normal boiling point in the required calculations.

Appendix D compares the results of the Guldberg approximation and the Lydersen method with literature values for 20 substances from the priority organic chemical list. The average absolute errors obtained by comparing calculated values with those from the literature are four and one per cent for the Guldberg approximation and the Lydersen method respectively. Although the Lydersen method is recommended for calculating the values used in the derivation of Soil Guideline Values, the Guldberg approximation is also a useful predictor of the critical point temperature.

2.4 Diffusion coefficient in air

2.4.1 Definition and use

Molecular diffusion is the net transport process of a molecule in a fluid as a result of intermolecular collisions rather than turbulence or bulk transport (Lyman *et al*. 1990). The diffusion coefficient or diffusivity of a chemical is the **proportionality constant**, D, in Equation 2-11, which expresses **Fick's first law** of diffusion (Mackay 2001). According to Lyman *et al*. (1990), the rate of diffusion is the property of two substances (that is, it depends not only on the chemical being transported but also on the medium through which the chemical moves).

Equation 2-11

$$N = -D_a A \frac{dC}{dy}$$

N	Flux of chemical, mol hr^{-1}
D_a	Diffusion coefficient or diffusivity of a chemical in air, m^2 hr^{-1}
A	Area, m^2
C	Concentration of diffusing chemical, mol m^{-3}
y	Distance in the direction of diffusion, m

The diffusion coefficient of a substance in air (D_a) is used in environmental models to predict how fast chemicals migrate through the environment from one media into another in the absence of any **advective** or bulk transport flow (Mackay 2001). Estimating the rate of diffusion of a chemical through porous materials including soil, sand and concrete are important in the CLEA software for estimating vapour transport of a chemical to indoor and outdoor air (Environment Agency 2008a).

2.4.2 Data availability and variability

Diffusion coefficients in air were not reported in the literature examined here for priority organic chemicals (see section 1.2.2). The CLEA software requires the diffusion coefficient in air in units of $m^2 s^{-1}$ (Environment Agency 2008b). Common unit conversions are presented in Table 2.6 (NIST 1995).

Table 2.6 Common unit conversions for diffusion coefficients in air (NIST 1995)

Converting from	To metres squared per second ($m^2 s^{-1}$)
$cm^2 s^{-1}$	Divide by 10 000
$cm^2 hr^{-1}$	Divide by 10 000, divide by 3 600
$m^2 hr^{-1}$	Divide by 3 600

2.4.3 Adjustments for temperature

Diffusion coefficients in air are dependent on temperature and pressure (Lyman *et al*. 1990). The methods for estimating the air diffusivity of a chemical in 2.4.4 include a temperature adjustment.

2.4.4 Methods for estimation

There are a number of methods for estimating the air diffusion coefficient of a substance and although the reported average errors are similar, several methods are applicable only to a limited number of chemical classes. Lyman *et al*. (1990) identified two methods that were relatively easy to apply, required only commonly available data, and reported good results for a wide range of general chemicals.

The Fuller, Schettler and Giddings (FSG) method is the easiest approach to apply and is reportedly applicable to non-polar gases at low and moderate temperatures (Lyman *et al*. 1990). It is also the method recommended by USEPA for modelling sub-surface hydrocarbon transport (USEPA 2006). Lyman *et al*. (1990) noted that the method is most accurate for chlorinated aliphatic chemicals and that aromatic, alkane, and ketone compounds deviate by plus or minus five per cent from measured values. Its accuracy is poorest with polar acids and glycols. The FSG method depends on the correlation shown in Equation 2-12 with the function of molecular weight (M_r) calculated using Equation 2-13.

Equation 2-12

$$D_a = \frac{0.001 T_{amb}^{1.75} \sqrt{M_r}}{P(V_A^{1/3} + V_B^{1/3})^2} \times \frac{1}{10000} m^2 cm^{-2}$$

D_a	Diffusion coefficient in air, $m^2 s^{-1}$
T_{amb}	Ambient soil temperature, K (= 283.15)
M_r	Function of molecular weight, mol g^{-1}
P	Ambient pressure, atm [= 1]
V_A	Molar volume of air, $cm^3 mol^{-1}$ [approximately 20.1, Lyman *et al*. 1990]
V_B	Molar volume of substance calculated using the Le Bas method, $cm^3 mol^{-1}$

Equation 2-13

$$M_r = \frac{M_A + M_B}{M_A M_B}$$

M_r	Function of molecular weight, mol g^{-1}
M_A	Molecular weight of air, g mol^{-1} [approximately 28.97, Lyman et al. 1990]
M_B	Molecular weight of substance, g mol^{-1}

The **molar volume** of a chemical (V_B) can be estimated from the density of the pure liquid at room temperature or from structural contributions using the LeBas method (Lyman *et al*. 1990, Montgomery 2007). Mackay *et al*. (2006) report the molar volume for a wide range of chemicals using the LeBas method.

The Wilke and Lee (WL) method for estimating the diffusion coefficient in air is reported to be usable over a wider range of compounds and temperatures than is the FSG method (Lyman *et al*. 1990). Across a range of chemical classes, Lyman *et al.* (1990) reported that the WL method was twice as accurate as the FSG method (that is, only a four per cent average absolute error compared with eight per cent for the latter). The WL method is significantly more accurate than the FSG method for nitriles, aromatic esters, and glycols (Lyman *et al*. 1990). The WL method requires knowledge of the normal boiling point of the chemical and is based on the correlation in Equation 2-14 with additional calculation steps shown in Equation 2-13, Equation 2-15, Equation 2-16, Equation 2-17, and Equation 2-18.

Equation 2-14

$$D_a = \frac{B' T_{amb}^{3/2} \sqrt{M_r}}{P \sigma_{AB}^{2} \Omega} \times \frac{1}{10000} m^2 cm^{-2}$$

D_a	Diffusion coefficient in air, m^2 s^{-1}
B’	Correlation coefficient (see Equation 2-15), unitless
T_{amb}	Ambient soil temperature, K (=283.15, Environment Agency 2008a)
M_r	Function of molecular weight (see Equation 2-13), mol g^{-1}
P	Ambient pressure, atm [1]
σ_{AB}	Characteristic length (see Equation 2-18), Å
Ω	Collision integral (see Equation 2-16), unitless

Equation 2-15

$$B' = 0.00217 - 0.00050\sqrt{\frac{1}{M_A} + \frac{1}{M_B}}$$

B’	Correlation coefficient, unitless
M_A	Molecular weight of air, g mol^{-1} [= 28.97, Lyman *et al*. 1990]
M_B	Molecular weight of substance, g mol^{-1}

Equation 2-16

$$\Omega = \frac{1.06036}{(T^*)^{0.15610}} + \frac{0.19300}{e^{0.47635T^*}} + \frac{1.03587}{e^{1.52996T^*}} + \frac{1.76474}{e^{3.89411T^*}}$$

Ω	Collision integral, unitless
T^*	Correlation coefficient (see Equation 2-17), unitless

Equation 2-17

$$T^* = \frac{T_{amb}}{\sqrt{(\varepsilon / k)_A (1.15 T_b)}}$$

T^*	Correlation coefficient, unitless
T_{amb}	Ambient soil temperature, K (= 283.15, Environment Agency 2008a)
$(\varepsilon/k)_A$	Function of the molecular energy of attraction and the Boltzmann constant for air, K (= 78.6, Lyman *et al*. 1990)
T_b	Boiling point, K

Equation 2-18

$$\sigma_{AB} = \frac{\sigma_A + 1.18 V_B^{1/3}}{2}$$

σ_{AB}	Average characteristic length of air and chemical, Å
σ_A	Characteristic length for air, Å [=3.711, Lyman *et al*. 1990]
V_B	Molar volume, $cm^3\ mol^{-1}$

Appendix E summarises the calculated diffusion coefficients in air at 10°C for the priority chemicals using the FSG and the WL method. The latter values are recommended for use in the derivation of Soil Guideline Values because of the method's reported accuracy compared to the FSG method (Lyman *et al*. 1990).

2.5 Diffusion coefficient in water

2.5.1 Definition and use

Molecular diffusion is the net transport process of a molecule in a fluid as a result of intermolecular collisions rather than turbulence or bulk transport (Lyman *et al*. 1990). The diffusion coefficient or diffusivity of a chemical is the proportionality constant, D, in Equation 2-19, which expresses **Fick's first law** of diffusion (Mackay 2001). According to Lyman *et al*. (1990), the rate of diffusion is the property of two substances (that is, it depends not only on the chemical being transported but also on the medium through which the chemical moves).

Equation 2-19

$$N = -D_w A \frac{dC}{dy}$$

N	Flux of chemical, $mol\ hr^{-1}$
D_w	Diffusion coefficient or diffusivity of a chemical in water, $m^2\ hr^{-1}$
A	Area, m^2
C	Concentration of diffusing chemical, $mol\ m^{-3}$
y	Distance in the direction of diffusion, m

The diffusion coefficient of a substance in water (D_w) is used in environmental models to predict how fast chemicals migrate through the environment from one media into another in the absence of any advective or bulk transport flow (Mackay 2001). Estimating the rate of diffusion of a chemical through saturated porous materials including plant material, soil, sand and concrete are important in the CLEA software for estimating plant uptake and vapour transport of a chemical to indoor and outdoor air (Environment Agency 2008a).

2.5.2 Data availability and variability

Diffusion coefficients in water were not commonly reported in the authoritative sources reviewed by this study. Montgomery (2007) provided the most comprehensive data with recommended values for 55 substances on the priority chemical list. However, Montgomery (2007) reported experimentally measured water diffusivity values for only 13 substances as shown in Table F1 in Appendix F. Most values were estimated using the Hayduk and Laudie (1974) method as described in 2.5.4. The CLEA software requires the diffusion coefficient in water in units of $m^2 s^{-1}$ (Environment Agency 2008b). Common unit conversions are presented in Table 2.7 (NIST 1995).

Table 2.7 Common unit conversions for diffusion coefficients in air (NIST 1995)

Converting from	To metre squared per second ($m^2 s^{-1}$)
$cm^2 s^{-1}$	Divide by 10,000
$cm^2 hr^{-1}$	Divide by 10,000, divide by 3,600
$m^2 hr^{-1}$	Divide by 3,600

2.5.3 Adjustments for temperature

Diffusion coefficients in water are probably dependent on temperature although diffusivity has not been sufficiently studied to draw firm conclusions (Lyman *et al*. 1990). The method for estimating the water diffusivity of a chemical in 2.5.4 includes a temperature adjustment for the viscosity of water.

2.5.4 Methods for estimation

The theoretically derived Stokes-Einstein equation is the foundation of many methods for estimating the diffusion coefficient of a chemical in a liquid (Lyman *et al*. 1990). The equation applies to large, spherical molecules diffusing through a solution of small molecules such as water. Deviations of chemical behaviour from that predicted by the Stokes-Einstein equation are reportedly due to variations in molecular size and shape (Lyman *et al*. 1990). An important limiting assumption in most methods for estimating water diffusivity is that diffusion occurs in an infinitely dilute solution, or at least where the concentration of the solute is less than 0.05 molar (Lyman *et al*. 1990).

Lyman *et al*. (1990) recommend the method proposed by Hayduk and Laudie for estimating water diffusivity as shown in Equation 2-20. Hayduk and Laudie (1974) reported an average absolute error of six per cent for 87 solutes diffusing into water, using the LeBas method for **molar volume** (V_B). V_B can also be estimated from the density of the pure liquid at room temperature (Montgomery 2007). Mackay *et al*. (2006) reported the molar volume for a wide range of chemicals using the LeBas method.

Equation 2-20

$$D_w = \frac{13.26 \times 10^{-5}}{\eta^{1.14} V_B^{\;0.589}} \quad \times \quad \frac{1}{10000} m^2 cm^{-2}$$

D_w	Diffusion coefficient in water, m^2 s^{-1}
η	Viscosity of water at 283.15K, cP [=1.307, Lyman *et al.* 1990]
V_B	Molar volume, cm^3 mol^{-1}

Table F1 in Appendix F contains a comparison between the diffusion coefficients in water derived using the Hayduk and Laudie method and experimental values reported by Montgomery (2007) for twelve priority organic chemicals. The average absolute error was 13 per cent, although the difference was as large as 75 per cent for benz[*a*]anthracene. Despite this, the Hayduk and Laudie (1974) method is still recommended for the derivation of Soil Guideline Values because of its general applicabililty, where the water diffusivity is required at 10°C. Table F2 in Appendix F summarises the recommended values for all priority organic chemicals.

2.6 Enthalpy of vapourisation

2.6.1 Definition and use

The enthalpy or heat of vapourisation (ΔH_v) is one of the fundamental thermodynamic properties of a substance. It is defined as the quantity of energy required to convert a unit mass of a liquid into a vapour without a rise in temperature (Lyman *et al.* 1990).

ΔH_v is temperature-dependant, decreasing in value as temperature increases (Lyman *et al.* 1990). Many estimation methods simplify this temperature dependence by using the enthalpy of vapourisation measured at the normal boiling point, where it is also termed $\Delta H_{v,b}$ or ΔH_b (Boethling and Mackay 2000; Lyman *et al.* 1990; USEPA 2001).

ΔH_v is important in modelling the environmental behaviour of organic compounds because it can be used to predict the temperature dependence of other physical-chemical properties including Henry's law constant (see 2.1.3) and vapour pressure (see 2.9.4).

2.6.2 Data availability and variability

Enthalpies of vapourisation were not commonly reported in the authoritative sources reviewed by this study. Lide (2008), Mackay *et al.* (2006), and NIST (2005) provided the enthalpy of vapourisation at normal boiling point for a limited number of the priority organic chemicals (see Table A3 in Appendix A). Although the difference between reported values was typically much less than one per cent, the highest reported difference was only 2.5 per cent.

The estimation methods in this report require the enthalpy of vapourisation of a chemical in units of J mol^{-1}. Common unit conversions are presented in Table 2.8 (NIST 1995).

Table 2.8 Common unit conversions for the enthalpy of vapourisation (NIST 1995)

Converting from	To joules per mole (J mol^{-1})
cal mol^{-1}	Multiply by 4.184
kJ mol^{-1}	Multiply by 1,000

2.6.3 Adjustments for temperature

The enthalpy of vapourisation does vary with temperature, decreasing in value as temperature increases (Lyman *et al*. 1990). Most values are reported or estimated at the normal boiling point (see also 2.6.4).

Boethling and Mackay (2000) recommend the Grain-Watson method for adjusting the enthalpy of vapourisation for temperatures lower than the boiling point. The method for liquids (and super-cooled liquids) uses the Clausius-Clapeyron equation presented in Equation 2-21. The proportionality constant, *m*, is calculated using Equation 2-22. This method requires that the boiling point (see 2.2), critical point temperature (see 2.3), and enthalpy of vaporisation at the normal boiling point of the chemical are known.

Equation 2-21

$$\Delta H_{v,amb} = \Delta H_b \left[\frac{(1 - T_{amb} / T_c)}{(1 - T_b / T_c)} \right]^m$$

$\Delta H_{v,amb}$	Enthalpy of vaporisation at the ambient temperature, J mol^{-1}
ΔH_b	Enthalpy of vaporisation at the normal boiling point, J mol^{-1}
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_b	Boiling point, K
T_c	Critical point temperature, K
m	Proportionality constant, dimensionless

Equation 2-22

$$m = 0.4133 - 0.2575 \frac{T_{amb}}{T_b}$$

m	Proportionality constant, dimensionless
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_b	Boiling point, K

2.6.4 Methods for estimation

Boethling and Mackay (2000) recommended the estimation method proposed by Fishtine (1963) to estimate ΔH_b. The Fishtine method considered the effects of molecular **van der Waals forces**, **dipole-dipole interactions** and **hydrogen bonding** on the enthalpy of vapourisation. Fishtine (1963) found that the enthalpy of vapourisation could be related to the chemical boiling point by accounting for these molecular interactions using an empirical constant as shown in Equation 2-23.

Equation 2-23

$$\Delta H_b = K_F T_b R \ln(82.06\ T_b)$$

ΔH_b	Enthalpy of vapourisation at normal boiling point, J mol^{-1}
K_F	Fishtine constant, dimensionless
T_b	Boiling point, K
R	Molar gas constant, J mol^{-1} K^{-1} [= 8.314472]

The Fishtine constant (K_F) is a dimensionless factor related to molecular structure and the **dipole moment**. Fishtine (1963) observed that for benzene derivatives with substantial dipole moments that do not form hydrogen bonds, K_F, was related to the dipole moment by Equation 2-24. Table 2.9 summarises molecular dipole moments for some of the benzene derivatives on the priority organic chemicals list (Lide 2008; Kim 2001). Boethling and Mackay (2000) also provide a table of Fishtine constants for a range of other aliphatic, alicyclic, and hydrogen-bonded aromatic organic compounds.

Equation 2-24

$$K_F = 1 + 0.02\mu$$

K_F	Fishtine constant, dimensionless
μ	Molecular dipole moment, Debye

In the absence of molecular dipole moment data for many **pesticides** based on aromatic molecular structures, an alternative method of deriving the enthalpy of vapourisation at normal boiling point is considered. Lyman *et al*. (1990) recommended the modified Klein method which is derived from the Clapeyron equation and requires the boiling point (see 2.2), critical point temperature (see 2.3) and critical pressure of the chemical. It is shown in Equation 2-25. The dimensionless Klein constant, K_{kl}, depends on boiling point as described in Table 2.10. The critical pressure is estimated from molecular structure using the Lydersen method described in Lyman *et al*. (1990).

Table G1 in Appendix G compares the estimated ΔH_b by using the Fishtine and modified Klein methods with those values reported in the literature for 29 priority organic chemicals. The average absolute errors for both methods were very similar at around five per cent, although there were significant deviations (over 30 per cent) for some chemicals including azinphos methyl, 2,4-dichlorophenol, and dieldrin. The modified Klein method is preferred for the derivation of Soil Guideline Values because of the lack of dipole moment measurements for many benzene derivatives on the priority chemicals list.

Table 2.9 Molecular dipole moments for several benzene derivatives (Lide 2008; Kim 2001)

Chemical	Dipole moment (Debye)
Benz[a]anthracene	0.067
Benzo[k]fluoranthene	0.092
Benzo[a]pyrene	0.049
Chlorobenzene	1.690
α-Chlorotoluene	1.820
2-Chlorotoluene	1.560
Chrysene	0.005
1,2-Dichlorobenzene	2.500
1,3-Dichlorobenzene	1.720
Ethylbenzene	0.590
Fluoranthene	0.220
Indeno[123-cd]pyrene	0.424
Naphthalene	0.009
Pyrene	0.013
Toluene	0.375
α,α,α-Trichlorotoluene	2.030
o-Xylene	0.640

Equation 2-25

$$\Delta H_b = RK_{kl}T_b \frac{\ln P_c \sqrt{1-1/[P_c(T_b/T_c)^3]}}{1-(T_b/T_c)} \quad x \quad 4.184\,J\,cal^{-1}$$

ΔH_b	Enthalpy of vapourisation at normal boiling point, J mol^{-1}
R	Molar gas constant, cal mol^{-1} K^{-1} [= 1.9872, Lyman *et al*. 1990]
K_{kl}	Klein constant, dimensionless
T_b	Boiling point, K
T_c	Critical point temperature, K
P_c	Critical pressure, atm [calculated using the Lydersen method in Lyman *et al*. 1990]

Table 2.10 Values for Klein Constant (Lyman *et al*. 1990)

Boiling point (K)	K_{kl} (dimensionless)
< 200	1.02
200 – 300	1.04
> 300	1.045

2.7 Octanol – water partition coefficient

2.7.1 Definition and use

The octanol-water partition coefficient, K_{ow}, is defined as the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of an octanol-water system (Lyman *et al*. 1990). K_{ow} is usually reported on a logarithmic scale, *log* K_{ow}, and the typical range varies from -3 to +7.

There are various experimental methods for determining K_{ow} in the laboratory (Boethling and Mackay 2000; Lyman et al. 1990). Note that the octanol-water partition coefficient is not the same as the ratio of a chemical's solubility in octanol to its solubility in water, because the octanol and aqueous phases in octanol/water system are not pure liquids (Lyman *et al*. 1990).

The octanol-water partition coefficient is a key parameter in understanding and predicting the environmental fate and transport behaviour of organic chemicals (Boethling and Mackay 2000; Lyman *et al*. 1990). K_{ow} is often used as a surrogate for the **lipophilicity** of a chemical and its tendency to concentrate in organic phases such as within plant lipids or fish from the aqueous solution (EU 2003; Mackay 2001). Chemicals with relatively low K_{ow} values are considered relatively **hydrophilic** and will tend to have high water solubilities and low bioconcentration factors (Lyman *et al*. 1990). It is also used in the prediction of other parameters including water solubility (see 2.10) and the organic carbon-water partition coefficient (see 2.8).

The $\log K_{ow}$ value of a chemical is required by the CLEA software to estimate the organic carbon-water partition coefficient, which determines the degree to which a chemical partitions between the soil and soil pore water. It is also used to predict the degree of partitioning of a chemical from water to plant cell lipids and determines the amount of uptake by fruit and vegetables (Environment Agency 2008a).

2.7.2 Data availability and variability

$\log K_{ow}$ values for organic chemicals are available in the literature (see Table A7 in Appendix A). There is considerable variability in the values reported (typically greater than five per cent) with the greatest variation observed for some **pesticides**, polycyclic aromatic hydrocarbons, and those organic chemicals where values vary due to the degree of **ionisation** at different pH values. K_{ow} and $\log K_{ow}$ values are dimensionless.

2.7.3 Adjustments for temperature

There are no temperature adjustments for this parameter.

Values of K_{ow} are normally measured at 20 or 25°C but the effect of temperature is very low, varying between 0.001 to 0.01 log K_{ow} units per °C (Lyman *et al*. 1990). There is no general trend for whether K_{ow} increases or decreases with increasing temperature.

2.7.4 Methods for estimation

Lyman *et al*. (1990) identified two different sets of methods to predict the octanol-water partition coefficient for a range of organic chemicals. The first group of methods required knowledge of the chemical structure, with K_{ow} determined by combining a number of fragment constants and structural factors (EU 2003; Lyman *et al*. 1990). The second group of methods were based around extrapolating from partitioning behaviour in other solvent-water systems using simple linear regression.

Boethling and Mackay (2000) noted the expanded and more sophisticated use of the fragment-based approaches to derive K_{ow} from molecular structure and reviewed several software programs developed for the PC to implement it. The EU *Technical Guidance Document on Risk Assessment* recommended cautious use of QSAR methods based on fragment approaches (EU 2003).

KOWWIN is published by the US Environmental Protection Agency and is available to download for free as part of the EPI software suite for most Windows-based PCs (USEPA 2008). Boethling and Mackay (2000) described the underlying methodology of this software as *reductionist*, meaning that the contribution of each molecular structural feature and interaction factor (such as the *ortho* interaction in benzenes) is evaluated by multiple regression analysis against a database of measured values. The fragments are relatively simple compared to those used in CLOGP (EU 2003). The key limitation in the accuracy of this method is therefore the size and coverage of the underlying database on which the methodology relies (Boethling and Mackay 2000).

CLOGP is a commercial software package for Windows-based PCs developed by BioByte Corporation, Claremont, California (BioByte 1999).[6] Boethling and Mackay (2000) described the approach behind CLOGP as *constructionist*; the fragment constants and interaction factors are built up from isolating these contributions in the simplest example molecules in which they occur. The procedure consists of two parts, the summation of fragments of each atom or functional group followed by the use of correction factors for features such as chain-length, ring size, and branching (EU 2003). The limitations of this method are the lack of data for some fragment types and the use of rigid rules to dissect molecular structure (Boethling and Mackay 2000).

Table H1 in Appendix H compares the recommended measured literature values for K_{ow} with the predictions of both KOWWIN and CLOGP. Both programs require the molecular structure to be entered in SMILES notation and this information was obtained for the priority organic chemicals by downloading the relevant 2D MOL files from the NIST Webbook (NIST 2005). Similar results were observed across the 64 priority organic chemicals for which measured values with CLOGP performed marginally better (absolute error of six per cent) than KOWWIN (absolute error of eight per cent).[7] Both estimation methods reported substantial errors from the measured values for dichlorvos and α,α,α-trichlorotoluene from 33 to 55 per cent. In the absence of a measured value for $\log k_{ow}$ the output from KOWWIN is recommended for the derivation of Soil Guideline Values because it is freely available.

2.8 Organic carbon-water partition coefficient

2.8.1 Definition and use

The soil-water partition coefficient, K_d, is a measure of the ratio of the amount of chemical adsorbed per unit mass of soil to its concentration in water at **equilibrium** (Boethling and Mackay 2000). It is influenced by many different chemical and soil factors including chemical concentration, solution pH, ionic strength and bulk solution chemistry, presence of suspended particulate or colloidal material, types and quantity of soil organic matter, clay mineral content, type and availability of surface **sorption** sites and bonding, and other chemical interactions at the soil-solution interface (Boethling and Mackay 2000; Lyman *et al*. 1990).

The organic carbon-water partition coefficient, K_{oc}, is the ratio of the amount of an organic chemical adsorbed per unit mass of organic carbon in the soil to its concentration at equilibrium in aqueous solution (Lyman *et al*. 1990). It is a more consistent measure of the extent to which organic chemicals partition between sorbed and dissolved phases and is used as a surrogate for the soil-water partition coefficient (K_d) in environmental modelling (Boethling and Mackay 2000; EU 2003; Mackay 2001). Studies by agricultural chemists have shown that organic chemicals tend to adsorb primarily to the organic matter present in soils (Mackay 2001).

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[6] CLOGP Version 4.0 is now part of the BIO-LOOM software suite (BioByte 2008)

[7] All margins of error based on comparison of log values

K_{oc} is often used to predict K_d by assuming a simple linear isotherm that in many cases will over estimate Kd by one or more orders of magnitude. In particular, the use of K_{oc} to predict K_d may not be appropriate where soils have a very low organic carbon content (less than 0.1 per cent) and/or a high mineral clay content or metal oxides, since the latter may have a dominant role in the sorption process (Boethling and Mackay 2000). In addition, the K_{oc} approach is only considered valid for neutral and relatively non-polar organic chemicals. Boethling and Mackay (2000) noted that polar acids and amines may correlate more readily with other properties such as cation exchange capacity, clay content, and total surface area for sorption, rather than organic matter content.

Sorption processes play a major role in determining the environmental fate and impact of organic chemicals (Boethling and Mackay 2000). K_{oc} is used in the CLEA software to determine the extent to which an organic chemical will partition between the sorbed, dissolved and vapour phases (Environment Agency 2008a).

2.8.2 Data availability and variability

Data on the organic carbon-water partition coefficient (K_{oc}) is available in the literature and reported from a wide range of studies (Montgomery 2007; Mackay *et al*. 2006). However, many of these studies have used widely varying experimental conditions including variations in soil and sediment type, organic matter type and content, chemical concentration, solution chemistry (pH, ionic strength, bulk chemistry), and other environmental parameters including temperature. Boethling and Mackay (2000) noted considerable difficulties in interpreting the results of such experimental studies, which are commonly cited with little experimental description, and in some cases are based on a single soil or sediment.

Therefore, unlike the other chemical properties described in this report, K_{oc} values for the priority organic chemicals have not been collated from the literature but are estimated from the octanol-water partition coefficient (K_{ow}) for use in generic risk assessments (see 2.8.4). The CLEA software requires the logarithm of K_{oc} of a chemical in units of $cm^3\ g^{-1}$ (Environment Agency 2008b). Common unit conversions are presented in Table 2.13 (NIST 1995).

Table 2.11 Common unit conversions for K_{oc} (NIST 1995)

Converting from	To cubic centimetre per gram ($cm^3\ g^{-1}$)
$L\ kg^{-1}$	No conversion necessary
$mL\ g^{-1}$	No conversion necessary
$m^3\ kg^{-1}$	Multiply by 1,000

2.8.3 Adjustments for temperature

The effect of temperature on the sorption of organic chemicals to soil is a measure of the strength of bonding involved (Boethling and Mackay 2000). The weaker the interaction between the organic chemical and soil, the less pronounced is the effect of temperature. Boethling and Mackay (2000) noted that in most cases, sorption at equilibrium decreases with increasing temperature but there are exceptions in the scientific literature. The methods for estimating the K_{oc} of a chemical in 2.8.4 do not include a temperature adjustment, but the datasets used to study this relationship are typically around room temperature.

2.8.4 Methods for estimation

Although there are methods based on molecular structure, the most widely applied approaches for estimating K_{oc} use empirical correlations with either the octanol-water partition coefficient (K_{ow}) or the aqueous solubility (Boethling and Mackay 2000; EU 2003). The literature contains many such relationships and selecting the most appropriate one depends on the quality and extent of the database used to develop the empirical model (Boethling and Mackay 2000). Empirical relationships are often developed for specific types or classes of organic chemical including alcohols, benzene and its derivatives, organic acids and esters, **pesticides**, phenols, polycyclic aromatic hydrocarbons, and triazines (Boethling and Mackay 2000; EU 2003).

EU (2003) developed its recommended list of empirical regression models from the work of Sabljic and co-workers (Sabljic and Gusten 1995; Sabljic *et al*. 1995), which used a hierarchical approach including general models (that is, **hydrophobic** and non-hydrophobic expressions), sub-general models (that is, phenol types, pesticides and so on), and class-specific models including alcohols, amides, nitro benzenes and triazines. Selected examples of these empirical linear regression equations are summarised in Table 2.12.

Table I1 in Appendix I summarises the calculated logarithm values of K_{oc} using the empirical models in Table 2.12. Where more than one method could be used to determine log K_{oc}, the more chemical specific approach is recommended to derive Soil Guideline Values. For example, in the case of phenol and the chlorophenols, the linear regression for phenols and nitro-benzenes only is preferred to the more general expression for non-hydrophobic compounds.

Table 2.12 Summary of selected linear regressions relating K_{oc} (cm^3 g^{-1}) to K_{ow} for different groups of organic chemicals (EU 2003; Sabljic and Gusten 1995)

Chemical group	Regression	Statistics[1]	Notes
Predominantly hydrophobics	$\log K_{oc} = 0.81 \log K_{ow} + 0.10$	n=81, r^2=0.89, s.e.=0.45	All chemicals containing, carbon, hydrogen, and the halogens
Non-hydrophobics	$\log K_{oc} = 0.52 \log K_{ow} + 1.02$	n=390, r^2=0.63, s.e.=0.56	All chemicals not classified as hydrophobics
Phenols, anilines, benzo-nitriles, nitrobenzenes	$\log K_{oc} = 0.63 \log K_{ow} + 0.90$	n=54, r^2=0.75, s.e.=0.40	Only with Cl, Br, OH, NO_2, CH_3, CH_3O, CF_3, NH_2, or OH as substituents
Pesticides	$\log K_{oc} = 0.47 \log K_{ow} + 1.09$	n=216, r^2=0.68, s.e.=0.43	Acetanilides, carbamates, esters, phenyl-ureas, phosphates, triazines, uracils
Phenols, benzo-nitriles	$\log K_{oc} = 0.57 \log K_{ow} + 1.08$	n=24, r^2=0.75, s.e.=0.37	Only with Cl, Br, NO_2, CH_3, CH_3O or OH as substituents
Phosphates	$\log K_{oc} = 0.49 \log K_{ow} + 1.17$	n=41, r^2=0.73, s.e.=0.45	
Triazines	$\log K_{oc} = 0.30 \log K_{ow} + 1.50$	n=16, r^2=0.32, s.e.=0.38	Only Cl, CH_3O, CH_3S, NH_2, N-alkyl as substituents

Note: [1] n = number of data; r^2 = correlation coefficient; s.e. = standard error of estimate

2.9 Vapour pressure

2.9.1 Definition and use

The vapour pressure of a substance is the pressure its vapour exerts in equilibrium with its pure liquid or solid phase (Boethling and Mackay 2000). It is an important parameter in understanding the transport and partitioning of a chemical between different environmental compartments (that is, between air, water, soil, and biota).

There are several direct and indirect experimental methods for determining vapour pressure (Boethling and Mackay 2000; Mackay *et al*. 2006). The greater challenge and larger experimental uncertainties are likely to be found in measuring vapour pressures less than one Pascal for essentially non-volatile substances. Temperature control in such experiments is essential because of the strong dependence of vapour pressure on temperature (Mackay *et al*. 2006).

It is often useful to determine the vapour pressure and other properties of a chemical by assuming that it is a liquid or super-cooled liquid at a temperature less than the melting point (Mackay *et al*. 2006). At very low environmental concentrations such as in liquid solutions or on aerosol particles, pure chemical behaviour relates to the liquid rather than the solid state.

Vapour pressure controls the volatility of a chemical from soil, and along with its water solubility, determines evaporation from water (Boethling and Mackay 2000). Predicting the volatility of a chemical in soil systems is important in the CLEA software for estimating chemical partitioning in the subsurface between sorbed phase, dissolved phase and gas phase (Environment Agency 2008a). It is an important parameter in estimating vapour transport of a chemical to indoor and outdoor air (Environment Agency 2008a).

2.9.2 Data availability and variability

Vapour pressure data for low boiling point organic chemicals are widely available in the scientific literature (see Table A8 in Appendix A). However, data for higher boiling point chemicals with low vapour pressures, such as polycyclic aromatic hydrocarbons, are rarer and likely to demonstrate greater variability (Boethling and Mackay 2000).

The CLEA software requires the vapour pressure of a chemical in units of Pa (Environment Agency 2008b). Common unit conversions are presented in Table 2.13 (NIST 1995).

Table 2.13 Common unit conversions for vapour pressure (NIST 1995)

Converting from	To Pascal (Pa)
atm	Multiply by 101,325
bar	Multiply by 100,000
mm Hg	Multiply by 133.3224
torr	Multiply by 133.3224

2.9.3 Adjustments for temperature

The vapour pressure of a chemical increases rapidly with temperature (Boethling and Mackay 2000). The fundamental relationship between equilibrium vapour pressure and temperature is described by the Clausius-Clapeyron equation (Boethling and Mackay 2000; Lyman *et al*. 1990; Mackay *et al*. 2006). The method for estimating the vapour pressure of a chemical in 2.9.4 includes a temperature adjustment based on the enthalpy of vapourisation (see 2.6).

2.9.4 Methods for estimation

Most of the estimation and correlation methods for estimating the vapour pressure of a chemical are designed for the greatest accuracy between the normal boiling point, T_b, and the critical point temperature (Lyman *et al*. 1990). Along with the Antoine Equation, the Grain-Watson method is recommended for estimating the vapour pressure of a liquid or super-cooled liquid, P_L, at temperatures less than the normal boiling point (Boethling and Mackay 2000; Lyman *et al*. 1990). As well as being able to consider the vapour pressure of solids, P_s, the Grain-Watson method is more reliable for higher boiling points (and therefore less volatile substances) than the Antoine equation.

Lyman *et al*. (1990) introduced a simplified form of the modified Watson correlation. Equation 2-26 is based on an integration of the Clausius-Clapeyron equation and requires that the boiling point (see 2.2) and the enthalpy of vapourisation at normal boiling point (see 2.6) are known. The proportionality constant, *m*, depends on whether the chemical is a solid or liquid at ambient temperature; its value is given in Table 2.14.

Equation 2-26

$$\ln\frac{P}{P_b}=\frac{\Delta H_b}{\Delta Z_b R T_b}\left[1-\frac{\left(3-2\frac{T_{amb}}{T_b}\right)^{m}}{\frac{T_{amb}}{T_b}}-2m\left(3-2\frac{T_{amb}}{T_b}\right)^{m-1}\ln\frac{T_{amb}}{T_b}\right]$$

P	Vapour pressure of the liquid (P_L) or solid (P_S) at ambient temperature, Pa
P_b	Vapour pressure at boiling point, Pa [= 101,325]
ΔH_b	Enthalpy of vapourisation at normal boiling point, J mol^{-1}
ΔZ_b	Compressibility factor, dimensionless [= 0.97, Lyman *et al*. 1990]
R	Molar gas constant, J mol^{-1} K^{-1} [= 8.314472]
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_b	Boiling point, K
m	Proportionality constant, dimensionless

Table 2.14 Values for constant *m* (Lyman *et al*. 1990)

	***m* (dimensionless)**
All liquids	0.19
Solids	
T_{amb} / T_b ratio < 0.5	1.19
0.5 ≤ T_{amb} / T_b ratio ≤ 0.6	0.80
T_{amb} / T_b ratio > 0.6	0.36

Boethling and Mackay (2000) described a further development of the Grain-Watson method for liquids as shown in Equation 2-27. One key difference between this newer method and the original one is the calculation of the constant, *m*, replacing the single value for liquids in Table 2.14 with a value found by using Equation 2-28.

Equation 2-27

$$\ln\frac{P_L}{P_b}=\frac{\Delta H_b}{RT_b}[1-\frac{(3-2\frac{T_{amb}}{T_b})^m}{\frac{T_{amb}}{T_b}}-2m(3-2\frac{T_{amb}}{T_b})^{m-1}\ln\frac{T_{amb}}{T_b}]$$

P_L	Vapour pressure of the liquid (P_L) at ambient temperature, Pa
P_b	Vapour pressure at boiling point, Pa [= 101,325]
ΔH_b	Enthalpy of vapourisation at normal boiling point, J mol^{-1}
R	Molar gas constant, J mol^{-1} K^{-1} [= 8.314472]
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_b	Boiling point, K
m	Proportionality constant, dimensionless

Equation 2-28

$$m=0.4133-0.2575\frac{T_{amb}}{T_b}$$

m	Proportionality constant, dimensionless
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_b	Boiling point, K

Perhaps the most important development in the Grain-Watson method described by Boethling and Mackay (2000) is the revised correction for solids. Equation 2-29 describes this new adjustment for the temperature dependence of the vapour pressure of a solid, P_S, with Equation 2-30 used to calculate the constant, *m'*. This method is analogous to the calculation for liquids and requires that the melting point of the chemical is known (Boethling and Mackay 2000). The vapour pressure of the solid, P_s, can be calculated by taking the exponent of Equation 2-29 and multiplying it by the vapour pressure of the liquid or super-cooled liquid, P_L, at the ambient temperature.

Equation 2-29

$$\ln\frac{P_S}{P_L}=0.6\ln(82.06\ T_m)[1-\frac{(3-2\frac{T_{amb}}{T_m})^{m'}}{\frac{T_{amb}}{T_m}}-2m'(3-2\frac{T_{amb}}{T_m})^{m'-1}\ln\frac{T_{amb}}{T_m}]$$

P_S	Vapour pressure of the solid (P_S) at ambient temperature, Pa
P_L	Vapour pressure at of the liquid (P_L) at ambient temperature, Pa
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_m	Melting point, K
m'	Proportionality constant, dimensionless

Equation 2-30

$$m' = 0.4133 - 0.2575 \frac{T_{amb}}{T_m}$$

m'	Proportionality constant, dimensionless
T_{amb}	Ambient soil temperature, K [= 283.15, Environment Agency 2008a]
T_m	Melting point, K

Table J1 in Appendix J compares the results of the modified Watson from Lyman *et al.* (1990) and the Grain-Watson method from Boethling and Mackay (2000) with the recommended literature values for vapour pressure at 20 or 25°C from Table A8 in Appendix A. The performance of both methods is similar for organic liquids with an appreciable vapour pressure with the majority of estimates within ten per cent of the literature value. Although most estimates of the very low vapour pressures of solids are only accurate to within an order of magnitude, the Grain-Watson method recommended by Boethling and Mackay (2000) is generally much more reliable than the older modified Watson method. The errors for both methods at very low vapour pressures are expected and are unlikely to have a substantial impact on environmental modelling (Boethling and Mackay 2000; Lyman *et al.* 1990). Table J2 in Appendix J summarises the calculated vapour pressures at 10°C for the priority chemicals using the Grain-Watson method. These values are recommended for deriving SGVs.

2.10 Water solubility

2.10.1 Definition and use

Water solubility is one of the most important properties for evaluating the fate and transport of a chemical in the environment (Boethling and Mackay 2000). It is a direct measure of chemical **lipophilicity**. Chemicals with high water solubility will partition readily and rapidly into the aqueous phase and will often remain in solution and be available for degradation. Chemicals that are sparingly soluble in water will often dissolve slowly into solution and partition more readily into other phases including air, solids, and the surface of solid particles including soil (Boethling and Mackay 2000).

Water solubility is used in the CLEA software to determine the maximum theoretical concentration of a chemical in the soil pore water and is a reality check on the linear partitioning approach used (Environment Agency 2008a). It is also important for estimating the air-water partitioning coefficient (K_{aw}), used to determine the partitioning behaviour of a chemical in the soil (see 2.1 for further discussion).

2.10.2 Data availability and variability

Water solubility data are widely available in the scientific literature and are typically reported at 20 or 25°C (see Table A9 in Appendix A). The data for sparingly soluble chemicals often shows the greatest variation, although this is still typically less than one order of magnitude. The IUPAC-NIST Solubility Database is a critically reviewed dataset including solubilities for many important contaminants at 10°C (IUPAC-NIST 2006). The CLEA software requires the water solubility of a chemical in units of mg L^{-1} (Environment Agency 2008b). Common unit conversions are presented in Table 2.15.

Table 2.15 Common unit conversions for water solubility

Converting from	To milligrams per litre (mg L^{-1})
ppb	Divide by 1,000
ppm	No conversion necessary
mol dm^{-3}	Multiply by molecular weight * 1,000
mmol L^{-1}	Multiply by molecular weight
µmol L^{-1}	Multiply by molecular weight, divide by 1,000
µg L^{-1}	Divide by 1,000
µg kg^{-1}	Divide by 1,000 [a]
mg kg^{-1}	No conversion necessary [a]
g/100g	Multiply by 10,000 [a]

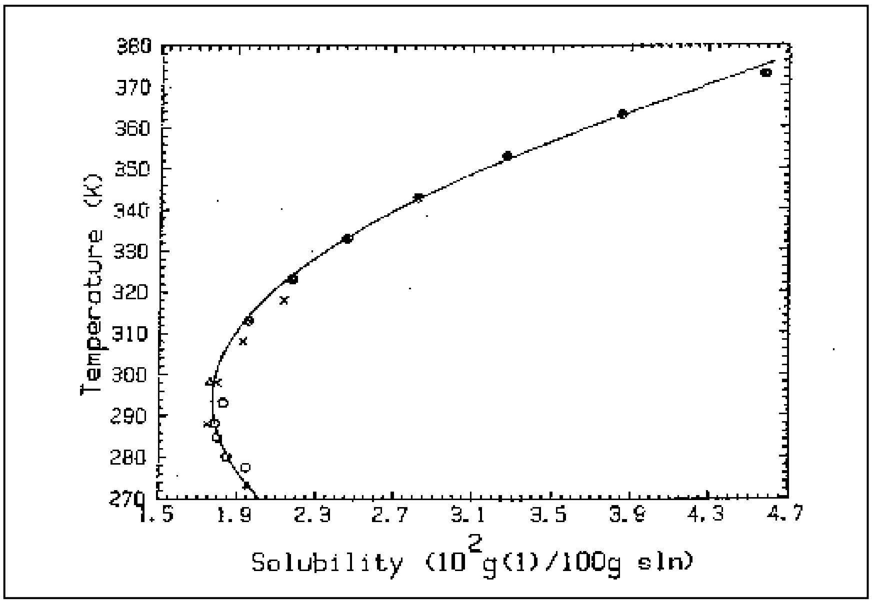
[a] Assumes that the density of water is approximately 1 kg L^{-1}.

2.10.3 Adjustments for temperature

Solubility is a function of temperature and it normally increases with increasing temperature (Boethling and Mackay 2000). However, not all solvation processes are **endothermic** and chemicals including oxygen and benzene may have a solubility minimum as a function of temperature; these can be shown as graphical plots of water solubility against temperature over the ambient temperature range (Boethling and Mackay 2000; IUPAC-NIST 2006). Figure 2-2 illustrates such a graphical plot for ethylbenzene.

Most experimental values for water solubility are measured at 20 or 25°C and the methods for estimating chemical solubility in 2.10.4 also assume a temperature of 25°C. In the absence of data at 10°C, values measured or calculated at 25°C may be used in the CLEA software. Table K1 in Appendix K presents a comparison between measured solubilities at 10 and 25°C for eighteen chemicals in the IUPAC-NIST Solubility Data (IUPAC-NIST 2006). Although the average absolute difference was only 13 per cent, the solubilities observed for 1,4-dichlorobenzene and naphthalene, which are both solids at room temperature with melting points less than 100°C, were about 60 per cent higher at 25°C. Care should therefore be taken when interpreting whether or not a chemical has reached its water solubility limit when evaluating the outputs from the CLEA software (Environment Agency 2008b).

Figure 2-2 Plot of experimental solubility data for ethylbenzene against temperature (after IUPAC-NIST 2006). (Reproduced from IUPAC-NIST Solubility Database, Version 1.0. 2006 by permission of IUPAC)



2.10.4 Methods for estimation

Boethling and Mackay (2000) recommended that general estimates of water solubility be obtained by using correlation with the octanol-water partition coefficient (K_{ow}) or a group contribution method derived from molecular structure.

Several researchers have reported a correlation between water solubility and K_{ow} for liquid chemicals at experimental temperatures (T_{exp}) of the general form, as shown in Equation 2-31 (Boethling and Mackay 2000). The parameters A and B are experimentally derived correlation constants. For chemicals that are solid at T_{exp}, Boethling and Mackay (2000) concluded that it is essential to correct the solubility calculation using the **fugacity ratio**. Applying **Walden's Rule** and assuming an experimental temperature of 25°C leads to Equation 2-32. This takes a more general form for finding solubility, where the chemical is in a solid or liquid state at 25°C, if the term (T_m – 298) can never be negative (that is, for liquids at 298K assume that the solid phase correction term is zero).

Equation 2-31

$$\log S_L = A - B \log K_{ow}$$

S_L	Water solubility of chemical in liquid physical state at experimental temperature (°C), mol L^{-1}
K_{ow}	Octanol-water partition coefficient, dimensionless
A	Experimental proportionality constant, mol L^{-1}
B	Experimental proportionality constant, mol L^{-1}

Equation 2-32

$$\log S_S = A - B\log K_{ow} - 0.01\,(T_m - 298)$$

S_S	Water solubility of chemical in solid physical state at 25°C, mol L^{-1}
K_{ow}	Octanol-water partition coefficient, dimensionless
A	Experimental proportionality constant, mol L^{-1}
B	Experimental proportionality constant, mol L^{-1}
T_m	Melting point, K

Note that the term (T_m – 298) cannot be less than zero. Negative values indicate that the chemical is present as a liquid and therefore the fugacity ratio term should be set to zero so that the overall equation takes the form of Equation 2-31.

Boethling and Mackay (2000) recommended that for general use, the experimental proportionality constants A and B have the values 1.10 and 1.25 respectively. This gives a generalised form of Equation 2-32 as shown in Equation 2-33. An improved correlation can be obtained by using the chemical class-specific values for A and B reported in the literature including alcohols, alkenes, benzene and its derivatives, halogenated hydrocarbons, esters, ketones and polycyclic aromatic hydrocarbons (Boethling and Mackay 2000; Lyman *et al*. 1990).

WSKOWIN is a computer program published by the US Environmental Protection Agency that incorporates the general form of Equation 2-33 but includes additional factors including molecular weight and empirically derived structural correction factors (Meylan *et al*. 1996; USEPA 2008). Equation 2-34 was derived from a dataset consisting of 1450 compounds with measured solubility, octanol-water partition coefficients, and melting points with an overall correlation coefficient (r^2) of 0.97 (USEPA 2008).

Equation 2-33

$$\log S \ = 1.10 - 1.25\log K_{ow} - 0.01\,(T_m - 298)$$

S	Water solubility at 25°C, mol L^{-1}
K_{ow}	Octanol-water partition coefficient, dimensionless
T_m	Melting point, K

Note that the term (T_m – 298) cannot be less than zero. Negative values indicate that the chemical is present as a liquid and therefore the fugacity ratio term should be set to zero so that the overall equation takes the form of Equation 2-31.

Equation 2-34

$$\log S \ = 0.693 - 0.96\log K_{ow} - 0.0092\,(T_m - 298) - 0.00314MW + corrections$$

S	Water solubility at 25°C, mol L^{-1}
K_{ow}	Octanol-water partition coefficient, dimensionless
T_m	Melting point, K
MW	Molecular mass, g mol^{-1}

Note that the term (T_m – 298) cannot be less than zero. Negative values indicate that the chemical is present as a liquid and therefore the fugacity ratio term should be set to zero.

The AQUAFAC group contribution method predicts water solubility from the molar activity coefficient (γ), which is a correction factor from ideal behaviour for solutes in real solutions (Atkins 1987; Myrdal *et al*. 1992). The general form of the calculation is shown in Equation 2-35 and incorporates the fugacity ratio term to correct for solids at 25°C. The group contribution, q_i, is obtained from a table of values and depends on its type (for example, -OH, $-NH_2$, $-CH_3$, -C=O, -Cl) and its bonding environment. Boethling and Mackay (2000) provide further guidance and a table of contribution values.

Equation 2-35

$$\log S = -0.01\,(T_m - 298) - \sum n_i q_i$$

S	Water solubility at 25°C, mol L^{-1}
T_m	Melting point, K
n_i	Number of times a chemical group appears in the molecule, dimensionless
q_i	Contribution of the chemical group to the molar activity coefficient, dimensionless

Table K2 in Appendix K compares the results of the modified K_{ow} correlation method, WSKOWIN, and the AQUAFAC contribution method with the recommended literature values for water solubility at 25°C from Table A9 in Appendix A. WSKOWIN required the molecular structure to be entered in SMILES notation and this information was obtained for the priority organic chemicals by downloading the relevant 2D MOL files from the NIST Webbook (NIST 2005).

The AQUAFAC and WSKOWIN methods performed marginally better than the general K_{ow} correlation for the priority organic chemicals, with almost all solubilities within one order of magnitude of the recommended literature value. However, the AQUAFAC method was applicable to fewer chemicals than the WSKOWIN method, the **pesticides** especially, because the group contributions from phosphate and some sulphur bond groups have not yet been defined.

Of those estimated values of the same order of magnitude or better, the AQUAFAC and the WSKOWIN method had an absolute error of 33 per cent. The K_{ow} method had an average error of 38 per cent for 43 chemicals, a slightly worse performance. In the absence of measured values, the WSKOWIN method is preferred to the other methods for deriving Soil Guideline Values, but the others are a reasonable alternative if the former is not applicable to the chemical of interest.

3 Recommended values

This chapter summarises the physical-chemical data for the priority organic chemicals in alphabetical order from aldrin to the isomers of xylene. Chemical properties are recommended from a review of the authoritative literature or by using one or more of the estimation methods described in Chapter 2. Additional information is provided on the identification and use of the chemicals.

3.1 Aldrin

Aldrin (CAS No. 309-00-2) is one of a number of persistent organochlorine pesticides banned from use in the UK (PSD 2008). It was used formerly as an **insecticide** and **fumigant** (Montgomery 1997). At **technical grade**, aldrin occurs as tan to dark brown crystals at room temperature with a mild chemical odour. It is readily metabolised to dieldrin (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values are shown in Table 3.1.

Table 3.1 Physical-chemical data for aldrin

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	5.79E-03	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.12E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.29E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.47	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.34 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	364.91 g mol^{-1}	Recommended literature value
Vapour pressure	1.35E-02 Pa	Estimated by Grain-Watson method
Water solubility	0.02 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{12}H_8Cl_6$	
Boiling point	657.8 K	Estimated by MP correlation method
Critical point temperature	986.7 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	45,721 J mol^{-1}	Estimated by Klein method
Henry's law constant	50.3 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	377.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.2 Atrazine

Atrazine (CAS No. 1912-24-9) is an **herbicide** based on a **triazine ring**. It has been used for the control of some annual grasses and broad-leaved weeds but now has restricted use in many countries including the UK (Montgomery 1997). It is a colourless powder or white crystalline solid at room temperature. The recommended physical-chemical data for the derivation of SGVs is shown in Table 3.2.

Table 3.2 Physical-chemical data for atrazine

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.81E-08	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.69E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.78E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.75	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.33 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	215.68 g mol^{-1}	Recommended literature value
Vapour pressure	3.93E-04 Pa	Estimated by Grain-Watson method
Water solubility	70 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_8H_{14}ClN_5$	
Boiling point	654.5 K	Estimated by MP correlation method
Critical point temperature	981.8 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	51,573 J mol^{-1}	Estimated by Klein method
Henry's law constant	2.88E-04 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	445.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.3 Azinphos-methyl

Azinphos-methyl (CAS No. 86-50-0) is a non-systemic **insecticide** based on a **triazine ring** (Montgomery 1997). It occurs as colourless crystals or a brown waxy solid at room temperature with a low odour threshold when dissolved in water. It is unstable at temperatures greater than 200°C (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.3.

Table 3.3 Physical-chemical data for azinphos-methyl

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.36E-11	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	4.40E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.61E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.69	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.31 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	317.32 g mol^{-1}	Recommended literature value
Vapour pressure	2.37E-09 Pa	Estimated by Grain-Watson method
Water solubility	9.5 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_{10}H_{12}N_3O_3PS_2$	
Boiling point	689.4 K	Estimated by MP correlation method
Critical point temperature	1034.1 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	96,650 J mol^{-1}	Recommended literature value
Henry's law constant	3.17E-04 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	346.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.4 Benzene

Benzene (CAS No. 71-43-2) is widely used in the manufacture of other chemicals including **polymers**, detergents, **pesticides**, pharmaceuticals, dyes, plastics, and resins, and as a **solvent** for waxes, resins, oils and natural rubber (MERCK 2006, Montgomery 2007). It is also an additive in petrol (MERCK 2006). It is a clear, colourless or slightly yellow liquid at room temperature with a distinctive aromatic or petrol-like odour (MERCK 2006). It is volatile and highly flammable. The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.4.

Table 3.4 Physical-chemical data for benzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.16E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	8.77E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	6.64E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.13	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.83 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	78.11 g mol^{-1}	Recommended literature value
Vapour pressure	6,240 Pa	Estimated by Grain-Watson method
Water solubility	1,780 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_6H_6	
Boiling point	353.2 K	Recommended literature value
Critical point temperature	562.0 K	Recommended literature value
Enthalpy of vaporisation at boiling point	30,720 J mol^{-1}	Recommended literature value
Henry's law constant	557 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	278.7 K	Recommended literature value
Physical state at room temperature	Liquid	

3.5 Benz[a]anthracene

Benz[a]anthracene (CAS No. 56-55-3) is also known as benzo[a]anthracene or 1,2-benzanthracene in the literature (Montgomery 2007). It is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification. It is a solid at room temperature, forming crystalline plates from glacial acetic acid or alcohol (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.5.

Table 3.5 Physical-chemical data for benz[a]anthracene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.16E-05	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	4.60E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.80E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.91	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.89 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	228.29 g mol^{-1}	Recommended literature value
Vapour pressure	1.24E-06 Pa	Estimated by Grain-Watson method
Water solubility	3.8E-03 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_{18}H_{12}$	
Boiling point	711.2 K	Recommended literature value
Critical point temperature	979.9 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	67,145 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.580 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	433.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.6 Benzo[b]fluoranthene

Benzo[b]fluoranthene (CAS No. 205-99-2) is also known as benz[e]acephenanthrylene, 2,3-benzfluoranthene, or 3,4-benzfluoranthene in the literature (Montgomery 2007). It is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification. The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.6.

Table 3.6 Physical-chemical data for benzo[b]fluoranthene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.05E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.36E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.62E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.08	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.02 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	252.31 g mol^{-1}	Recommended literature value
Vapour pressure	6.34E-08 Pa	Estimated by Grain-Watson method
Water solubility	2.0E-03 mg L^{-1} (20°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{20}H_{12}$	
Boiling point	754.2 K	Recommended literature value
Critical point temperature	1021.1 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	72,435 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.051 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	441.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.7 Benzo[k]fluoranthene

Benzo[k]fluoranthene (CAS No. 207-08-9) is also known as 8,9-benzofluoranthene, 11,12-benzofluoranthene, or dibenzo[bjk]fluorene in the literature (Montgomery 2007). It is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification. The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.7.

Table 3.7 Physical-chemical data for benzo[k]fluoranthene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.74E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.36E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.62E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.26	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.17 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	252.31 g mol^{-1}	Recommended literature value
Vapour pressure	1.64E-08 Pa	Estimated by Grain-Watson method
Water solubility	8.0E-04 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{20}H_{12}$	
Boiling point	753.2 K	Recommended literature value
Critical point temperature	1019.8 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	72,328 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.043 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	490.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.8 Benzo[ghi]perylene

Benzo[ghi]perylene (CAS No. 191-24-2) is also known as 1,12-benzoperylene in the literature (Montgomery 2007). It is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification. The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.8.

Table 3.8 Physical-chemical data for benzo[ghi]perylene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.36E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.22E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.56E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.81	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.62 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	276.33 g mol^{-1}	Recommended literature value
Vapour pressure	1.55E-10 Pa	Estimated by Grain-Watson method
Water solubility	2.6E-04 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{22}H_{12}$	
Boiling point	798.2 K	Recommended literature value
Critical point temperature	1063.6 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	77,997 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.075 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	545.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.9 Benzo[a]pyrene

Benzo[a]pyrene (CAS No. 50-32-8) is also known as 1,2-benzopyrene, 1,4-benzopyrene, or B(a)P in the literature (Montgomery 2007). It is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification. Benzo[a]pyrene is a solid at room temperature forming yellow plate or needle shaped crystals when precipitated from a mixture of benzene and methanol (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.9.

Table 3.9 Physical-chemical data for benzo[a]pyrene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.76E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.38E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.67E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.18	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.11 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	252.31 g mol^{-1}	Recommended literature value
Vapour pressure	2.0E-08 Pa	Estimated by Grain-Watson method
Water solubility	3.8E-03 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{20}H_{12}$	
Boiling point	768.2 K	Recommended literature value
Critical point temperature	1040.1 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	73,770 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.046 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	454.3 K	Recommended literature value
Physical state at room temperature	Solid	

3.10 Carbon disulphide

Carbon disulphide (CAS No. 75-15-0) is also known as carbon bisulphide in the literature (Montgomery 2007).[8] It is an industrial **solvent** used in the production of **polymers** such as rayon and viscose and in other products such as enamels, paints, and varnishes (MERCK 2006). It has also been used as an **herbicide** and a grain fumigant (Montgomery 2007). At **technical grade**, it is a clear, colourless to pale yellow liquid at room temperature with a strong odour like rotten vegetables. Carbon disulphide is highly flammable and very slowly decomposes on standing (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.10.

Table 3.10 Physical-chemical data for carbon disulphide

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	4.08E-01	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	1.04E-05 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	8.28E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.00	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.06 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	76.14 g mol^{-1}	Recommended literature value
Vapour pressure	26,500 Pa	Estimated by Grain-Watson method
Water solubility	2,100 mg L^{-1} (20°C)	Recommended literature value
Other useful data		
Chemical formula	CS_2	
Boiling point	319.2 K	Recommended literature value
Critical point temperature	552.0 K	Recommended literature value
Enthalpy of vaporisation at boiling point	26,740 J mol^{-1}	Recommended literature value
Henry's law constant	1750 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	161.7 K	Recommended literature value
Physical state at room temperature	Liquid	

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[8] In American literature, sulphide is written as sulfide.

3.11 Chlorobenzene

Chlorobenzene (CAS No. 108-90-7) is used in the manufacture of other chemicals including phenol, chloronitrobenzenes, and aniline, and as a **solvent** for **pesticides**, paints and dyes (MERCK 2006, Montgomery 2007). Other common names include benzene chloride and monochlorobenzene (MERCK 2006). It is a clear, colourless, flammable liquid at room temperature with a distinctive sweet almond or moth-ball like odour. **Technical grades** of chlorobenzene may contain minor quantities of benzene and dichlorobenzene (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.11.

Table 3.11 Physical-chemical data for chlorobenzene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.31E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.57E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.92E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.84	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.40 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	112.56 g mol^{-1}	Recommended literature value
Vapour pressure	673 Pa	Estimated by Grain-Watson method
Water solubility	387 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_6H_5Cl	
Boiling point	404.9 K	Recommended literature value
Critical point temperature	633.4 K	Recommended literature value
Enthalpy of vaporisation at boiling point	35,190 J mol^{-1}	Recommended literature value
Henry's law constant	367 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	227.8 K	Recommended literature value
Physical state at room temperature	Liquid	

3.12 Chloroethene

Chloroethene (CAS No. 75-01-4) is also commonly known as vinyl chloride or chloroethylene (MERCK 2006, Montgomery 2007). It is used in the manufacture of polyvinyl chloride and co-**polymers** as well as adhesives, and as a refrigerant and **solvent**. It is a colourless, flammable, liquefied compressed gas at room temperature, with a faint, sweetish odour that **polymerises** in the presence of light (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.12.

Table 3.12 Physical-chemical data for chloroethene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	7.47E-01	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	1.11E-05 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	8.34E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	1.38	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.22 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	62.50 g mol^{-1}	Recommended literature value
Vapour pressure	2.20E+05 Pa	Estimated by Grain-Watson method
Water solubility	2,760 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_2H_3Cl	
Boiling point	259.4 K	Recommended literature value
Critical point temperature	432.0 K	Recommended literature value
Enthalpy of vaporisation at boiling point	20,800 J mol^{-1}	Recommended literature value
Henry's law constant	2,690 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	119.4 K	Recommended literature value
Physical state at room temperature	Liquid / gas	

3.13 2-Chlorophenol

2-Chlorophenol (CAS No. 95-57-8) or ortho-chlorophenol is used as a component of disinfectants, a solvent for polyester fibres, and an intermediate in the manufacture of phenolic resins (Montgomery 2007). It is a pale amber-coloured liquid at room temperature with a medicinal odour (MERCK 2006). It is a weak acid (pK_a around 8.5) with around three per cent ionised in solution at pH 7 (Mackay *et al*. 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.13.

Table 3.13 Physical-chemical data for 2-chlorophenol

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.35E-04	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	7.14E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.71E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.15	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.31 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	128.56 g mol^{-1}	Recommended literature value
Vapour pressure	79.6 Pa	Estimated by Grain-Watson method
Water solubility	22,700 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_6H_4ClOH	
Boiling point	448.1 K	Recommended literature value
Critical point temperature	670.8 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	40,050 J mol^{-1}	Recommended literature value
Henry's law constant	0.653 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	282.6 K	Recommended literature value
Physical state at room temperature	Liquid	

3.14 α-Chlorotoluene

α-Chlorotoluene (CAS No. 100-44-7) is used in the manufacture of perfumes, pharmaceuticals, dyes and resins (MERCK 2006). It is also commonly known as benzyl chloride or (chloromethyl) benzene. It is a liquid at room temperature with an unpleasant, irritating odour. The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.14.

Table 3.14 Physical-chemical data for α-chlorotoluene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	7.47E-03	Estimated by Clapeyron relationship from the Henry's law constant at 20°C
Diffusion coefficient in air	6.81E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.34E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.30	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.96 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	126.58 g mol^{-1}	Recommended literature value
Vapour pressure	68.5 Pa	Estimated by Grain-Watson method
Water solubility	493 mg L^{-1} (20°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_5CH_2Cl$	
Boiling point	452.2 K	Recommended literature value
Critical point temperature	685.8 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	40,188 J mol^{-1}	Estimated by Klein method
Henry's law constant	36 Pa $m^3\ mol^{-1}$ (20°C)	Recommended literature value
Melting point	228.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.15 2-Chlorotoluene

2-Chlorotoluene (CAS No. 95-49-8) is used as an industrial **solvent** and in the manufacture of dyes (MERCK 2006). It is also commonly known as ortho-chlorotoluene or 1-chloro-2-methylbenzene. It is a liquid at room temperature. The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.15.

Table 3.15 Physical-chemical data for 2-chlorotoluene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.47E-02	Estimated by Clapeyron relationship from the Henry's law constant at 20°C
Diffusion coefficient in air	6.88E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.34E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.42	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.87 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	126.58 g mol^{-1}	Recommended literature value
Vapour pressure	201 Pa	Estimated by Grain-Watson method
Water solubility	117 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_7H_7Cl	
Boiling point	432.2 K	Recommended literature value
Critical point temperature	655.5 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	37,500 J mol^{-1}	Recommended literature value
Henry's law constant	295 Pa $m^3\ mol^{-1}$ (20°C)	Recommended literature value
Melting point	237.4 K	Recommended literature value
Physical state at room temperature	Liquid	

3.16 Chrysene

Chrysene or 1,2-benzphenanthrene (CAS No. 218-01-9) is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification (Montgomery 2007). Chrysene is a solid at room temperature forming plate-shaped crystals when precipitated from benzene (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.16.

Table 3.16 Physical-chemical data for chrysene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.18E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.57E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.77E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.73	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.74 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	228.29 g mol^{-1}	Recommended literature value
Vapour pressure	4.52E-08 Pa	Estimated by Grain-Watson method
Water solubility	0.002 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{18}H_{12}$	
Boiling point	721.2 K	Recommended literature value
Critical point temperature	993.7 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	68,085 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.065 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	528.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.17 DDT

DDT (p,p'-DDT CAS No. 50-29-3; o,p'-DDT CAS No. 789-02-6) was used widely as a **pesticide** and is one of a number of persistent organochlorine pesticides now banned from use in the UK (PSD 2008, Montgomery 2007). It occurs as white crystals or a waxy solid at room temperature with a faint, aromatic-like odour (Montgomery 2007). It is resistant to destruction by light and oxidation and its unusual stability has resulted in its residues being difficult to remove from water, soil and foods (MERCK 2006). The **technical grade** typically contains 77 per cent p,p'-DDT by weight and 15 per cent o,p'-DDT (Montgomery 2007). The recommended physical-chemical data of p,p'-DDT for the derivation of Soil Guideline Values is shown in Table 3.17.

Table 3.17 Physical-chemical data for p,p'-DDT

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.17E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.22E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.19E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.11	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.05 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	354.49 g mol^{-1}	Recommended literature value
Vapour pressure	6.06E-02 Pa	Estimated by Grain-Watson method
Water solubility	5.7E-03 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{14}H_9Cl_5$	
Boiling point	533.2 K	Recommended literature value
Critical point temperature	717.1 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	50,740 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.903 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	381.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.18 Dibenz[ah]anthracene

Dibenz[ah]anthracene or 1,2:5,6-dibenzanthracene (CAS No. 53-70-3) is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification (Montgomery 2007). It occurs as colourless to pale yellow crystals at room temperature with a faint, pleasant odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.18.

Table 3.18 Physical-chemical data for dibenz[ah]anthracene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	5.40E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.08E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.40E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	6.38	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	5.27 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	278.35 g mol^{-1}	Recommended literature value
Vapour pressure	1.66E-10 Pa	Estimated by Grain-Watson method
Water solubility	6.0E-04 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{22}H_{14}$	
Boiling point	797.2 K	Recommended literature value
Critical point temperature	1062.3 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	78,120 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.172 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	542.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.19 1,2-Dichlorobenzene

1,2-Dichlorobenzene or ortho-dichlorobenzene (CAS No. 95-50-1) is used as an industrial **solvent**, degreasing agent, **fumigant**, and an intermediate in dye manufacture (MERCK 2006, Montgomery 2007). It is a clear, colourless to pale yellow liquid at room temperature with a pleasant, aromatic and grassy odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.19.

Table 3.19 Physical-chemical data for 1,2-dichlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.38E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	6.75E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.37E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.38	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.84 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	147.00 g mol^{-1}	Recommended literature value
Vapour pressure	72.1 Pa	Estimated by Grain-Watson method
Water solubility	133 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_6H_4Cl_2$	
Boiling point	453.7 K	Recommended literature value
Critical point temperature	690.6 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	39,660 J mol^{-1}	Recommended literature method
Henry's law constant	195 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	256.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.20 1,3-Dichlorobenzene

1,3-Dichlorobenzene or meta-dichlorobenzene (CAS No. 541-73-1) is used as a **fumigant** and **insecticide** (Montgomery 2007). It is a clear, colourless liquid at room temperature with a disinfectant or musty-like odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.20.

Table 3.20 Physical-chemical data for 1,3-dichlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.61E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	6.77E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.37E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.48	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.92 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	147.00 g mol^{-1}	Recommended literature value
Vapour pressure	109 Pa	Estimated by Grain-Watson method
Water solubility	103 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_6H_4Cl_2$	
Boiling point	446.2 K	Recommended literature value
Critical point temperature	685.7 K	Recommended literature value
Enthalpy of vaporisation at boiling point	38,620 J mol^{-1}	Recommended literature value
Henry's law constant	318 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	248.4 K	Recommended literature value
Physical state at room temperature	Liquid	

3.21 1,4-Dichlorobenzene

1,4-Dichlorobenzene or para-dichlorobenzene (CAS No. 106-46-7) is used as a moth and bird repellent, **fumigant** and **germicide**, a deodorizer, and in the manufacture of dyes, pharmaceuticals and disinfectants (Montgomery 2007). It occurs as colourless to white crystals at room temperature with a sweet, mothball and almond-like odour (Montgomery 2007). It **sublimes** at ambient temperatures (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.21.

Table 3.21 Physical-chemical data for 1,4-dichlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	4.70E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	6.77E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.37E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.40	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.85 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	147.00 g mol^{-1}	Recommended literature value
Vapour pressure	38.5 Pa	Estimated by Grain-Watson method
Water solubility	51.2 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_6H_4Cl_2$	
Boiling point	447.2 K	Recommended literature value
Critical point temperature	680.7 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	38,790 J mol^{-1}	Recommended literature value
Henry's law constant	244 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	326.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.22 1,2-Dichloroethane

1,2-Dichloroethane or 1,2-DCA (CAS No. 107-06-2) is used in the manufacture of other chlorinated hydrocarbons, as an **antiknock agent** in petrol, as a **solvent** in paints, varnishes, metal degreasing, soaps and scouring compounds, and as a soil and food **fumigant** (Montgomery 2007). It is one of a number of persistent organochlorine **pesticides** banned from use in the UK (PSD 2008). It is a clear, colourless, oily liquid at room temperature with a pleasant, chloroform-like odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.22.

Table 3.22 Physical-chemical data for 1,2-dichloroethane

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.38E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	8.60E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	6.74E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	1.48	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.30 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	98.96 g mol^{-1}	Recommended literature value
Vapour pressure	4920 Pa	Estimated by Grain-Watson method
Water solubility	8,680 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_2H_4Cl_2$	
Boiling point	356.7 K	Recommended literature value
Critical point temperature	561.0 K	Recommended literature value
Enthalpy of vaporisation at boiling point	31,980 J mol^{-1}	Recommended literature value
Henry's law constant	121 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	237.5 K	Recommended literature value
Physical state at room temperature	Liquid	

3.23 2,4-Dichlorophenol

2,4-Dichlorophenol (CAS No. 120-83-2) is used as an intermediate in the manufacture of **pesticides**, antiseptics and seed disinfectants (MERCK 2006, Montgomery 2007). It is a solid at room temperature with colourless to yellow crystals with a sweet, musty, or medicinal odour (Montgomery 2007). It is a weak acid (pK_a of around eight) with around 10 per cent ionised in solution at pH 7 (Mackay *et al*. 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.23.

Table 3.23 Physical-chemical data for 2,4-dichlorophenol

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	5.07E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	6.46E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.21E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.23	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.92 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	163.00 g mol^{-1}	Recommended literature value
Vapour pressure	25.4 Pa	Estimated by Grain-Watson method
Water solubility	4,500 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_3Cl_2OH$	
Boiling point	483.2 K	Recommended literature value
Critical point temperature	709.7 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	36,780 J mol^{-1}	Recommended literature value
Henry's law constant	0.327 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	318.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.24 Dichlorvos

Dichlorvos (CAS No. 62-73-7) is an organophosphorus **insecticide** and **fumigant** against flies, mosquitoes and moths (Montgomery 1997). It is a colourless to yellow liquid at room temperature with an aromatic odour (Montgomery 1997). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.24.

Table 3.24 Physical-chemical data for dichlorvos

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.51E-07	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.91E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.79E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	1.34	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.83 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	220.98 g mol^{-1}	Recommended literature value
Vapour pressure	2.95 Pa	Estimated by Grain-Watson method
Water solubility	16,000 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_4H_7Cl_2O_4P$	
Boiling point	507.2 K	Recommended literature value
Critical point temperature	760.8 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	47,546 J mol^{-1}	Estimated by Fishtine method
Henry's law constant	5.59E-03 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point		
Physical state at room temperature	Liquid	

3.25 Dieldrin

Dieldrin (CAS No. 60-57-1) is one of a number of persistent organochlorine pesticides banned from use in the UK (PSD 2008). It was used as an **insecticide** and in the wool-processing industry (Montgomery 2007). Dieldrin is a **stereoisomer** of endrin and occurs as either white crystals or pale tan-coloured flakes at room temperature with little or no odour (Montgomery 1997). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.25.

Table 3.25 Physical-chemical data for dieldrin

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.73E-04	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.03E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.28E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.94	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.59 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	380.91 g mol^{-1}	Recommended literature value
Vapour pressure	4.18E-08 Pa	Estimated by Grain-Watson method
Water solubility	0.2 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{12}H_8Cl_6O$	
Boiling point	710.0 K	Estimated by MP correlation method
Critical point temperature	1065.0 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	76,600 J mol^{-1}	Recommended literature value
Henry's law constant	5.88 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	448.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.26 α-Endosulfan

α-Endosulfan or endosulfan I (CAS No. 959-98-8) is an **insecticide** used on vegetable crops (Montgomery 1997). It occurs as colourless to brown crystals or flakes at room temperature with a sulphurous odour (Montgomery 1997). Commercially used products are actually a mixture of the α-isomer and β-isomer (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.26.

Table 3.26 Physical-chemical data for α-endosulfan

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.89E-03 (25°C)	Estimated by direct calculation from water solubility and vapour pressure at 25°C
Diffusion coefficient in air	4.08E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.31E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.69	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.94 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	406.93 g mol^{-1}	Recommended literature value
Vapour pressure	6.11E-03 Pa (25°C)	Recommended literature value
Water solubility	0.53 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_9H_6Cl_6O_3S$	
Boiling point	690.4 K	Estimated by MP correlation method
Critical point temperature	1035.6 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point		
Henry’s law constant	7.68 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	379.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.27 β-Endosulfan

β-Endosulfan or endosulfan II (CAS No. 33213-65-9) is an **insecticide** used on vegetable crops (Montgomery 1997). It occurs as colourless to brown crystals or flakes at room temperature with a sulphurous odour (Montgomery 1997). Commercially used products are actually a mixture of the α-isomer and β-isomer (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.27.

Table 3.27 Physical-chemical data for β-endosulfan

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.88E-03 (25°C)	Estimated by direct calculation from water solubility and vapour pressure at 25°C
Diffusion coefficient in air	4.01E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.31E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.62	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.90 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	406.93 g mol^{-1}	Recommended literature value
Vapour pressure	3.20E-03 Pa (25°C)	Recommended literature value
Water solubility	0.28 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_9H_6Cl_6O_3S$	
Boiling point	742.4 K	Estimated by MP correlation method
Critical point temperature	1113.6 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point		
Henry's law constant	5.12 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	481.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.28 Ethylbenzene

Ethylbenzene (CAS No. 100-41-4) is an important chemical intermediate in the production of many compounds including styrene, benzoic acid and phenylethanes, and as an industrial **solvent** (Montgomery 2007). It is a clear, colourless, flammable liquid at room temperature with a sweet petrol-like odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.28.

Table 3.28 Physical-chemical data for ethylbenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.39E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.04E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.31E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.15	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.65 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	106.17 g mol^{-1}	Recommended literature value
Vapour pressure	553 Pa	Estimated by Grain-Watson method
Water solubility	180 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_8H_{10}	
Boiling point	409.4 K	Recommended literature value
Critical point temperature	617.2 K	Recommended literature value
Enthalpy of vaporisation at boiling point	35,570 J mol^{-1}	Recommended literature value
Henry's law constant	843 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	178.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.29 Fenitrothion

Fenitrothion (CAS No. 122-14-5) is an **insecticide** (MERCK 2006). It is a yellow oil at room temperature (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.29.

Table 3.29 Physical-chemical data for fenitrothion

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.60E-06 (20°C)	Estimated by direct calculation from water solubility and vapour pressure at 20°C
Diffusion coefficient in air	4.90E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.97E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.44	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.86 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	277.23 g mol^{-1}	Recommended literature value
Vapour pressure	8.00E-04 Pa (20°C)	Recommended literature value
Water solubility	25.3 mg L^{-1} (20°C)	Recommended literature value
Other useful data		
Chemical formula	$C_9H_{12}NO_5PS$	
Boiling point	606.5 K	Estimated by MP correlation method
Critical point temperature	909.8 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point		
Henry's law constant	0.095 Pa m^3 mol^{-1} (20°C)	Recommended literature value
Melting point	276.6 K	Recommended literature value
Physical state at room temperature	Liquid	

3.30 Fluoranthene

Fluoranthene, 1,2-benzacenaphthene or benzo[jk]fluorene (CAS No. 206-44-0) is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification (Montgomery 2007). Fluoranthene is a solid at room temperature forming colourless to light yellow crystals at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.30.

Table 3.30 Physical-chemical data for fluoranthene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.29E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.01E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.11E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.13	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.26 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	202.25 g mol^{-1}	Recommended literature value
Vapour pressure	1.31E-04 Pa	Estimated by Grain-Watson method
Water solubility	0.23 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{16}H_{10}$	
Boiling point	657.2 K	Recommended literature value
Critical point temperature	923.0 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	60,826 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.96 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	383.3 K	Recommended literature value
Physical state at room temperature	Solid	

3.31 Hexachlorobenzene

Hexachlorobenzene or perchlorobenzene (CAS No. 118-74-1) is one of a number of persistent organochlorine **pesticides** banned from use in the UK (PSD 2008). It is also used in the manufacture of pentachlorophenol and as a wood preservative (Montgomery 2007). It forms colourless or white **monoclinic** crystals at room temperature that **sublime** on heating (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.31.

Table 3.31 Physical-chemical data for hexachlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.04E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.99E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.06E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.47	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.53 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	284.78 g mol^{-1}	Recommended literature value
Vapour pressure	8.69E-05 Pa	Estimated by Grain-Watson method
Water solubility	9.60E-03 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_6Cl_6	
Boiling point	597.7 K	Recommended literature value
Critical point temperature	845.7 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	56,010 J mol^{-1}	Estimated by Klein method
Henry's law constant	131 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	502.0 K	Recommended literature value
Physical state at room temperature	Solid	

3.32 Hexachloro-1,3-butadiene

Hexachlorobutadiene (CAS No. 87-68-3) is an industrial **solvent**, heat transfer liquid, vineyard **fumigant**, and chemical intermediate for fluorinated lubricants and rubber compounds (MERCK 2006, Montgomery 2007). It is a clear, yellow-green liquid with a faint turpentine-like odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.32.

Table 3.32 Physical-chemical data for hexachloro-1,3-butadiene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.55E-01	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.40E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.23E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.86	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.04 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	260.76 g mol^{-1}	Recommended literature value
Vapour pressure	33 Pa	Estimated by Grain-Watson method
Water solubility	4.8 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_4Cl_6	
Boiling point	488.2 K	Recommended literature value
Critical point temperature	741.3 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	38,721 J mol^{-1}	Estimated by Klein method
Henry's law constant	1030 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	252.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.33 α-Hexachlorocyclohexane

α-Hexachlorocyclohexane (HCH), α-benzene hexachloride, α-lindane, or α-BHC (CAS No. 319-84-6) is an **insecticide** (Montgomery 1997). α-Hexachlorocyclohexane is a **stereoisomer** of the active ingredient of lindane (Montgomery 2007). HCH containing less than 99 per of the gamma **isomer** is banned from use in the UK (PSD 2008). It forms a brownish-white crystalline solid at room temperature with a phosgene-like odour (Montgomery 1997). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.33.

Table 3.33 Physical-chemical data for α-hexachlorocyclohexane

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.11E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.84E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.84E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.77	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.15 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	290.83 g mol^{-1}	Recommended literature value
Vapour pressure	6.47E-03 Pa	Estimated by Grain-Watson method
Water solubility	2 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_6Cl_6$	
Boiling point	561.2 K	Recommended literature value
Critical point temperature	789.6 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	51,134 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.872 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	431.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.34 β-Hexachlorocyclohexane

β-Hexachlorocyclohexane, β-benzene hexachloride, β-lindane, or β-BHC (CAS No. 319-85-7) is an **insecticide** (Montgomery 1997). β-Hexachlorocyclohexane is a **stereoisomer** of the active ingredient of lindane (Montgomery 2007). HCH containing less than 99 per of the gamma **isomer** is banned from use in the UK (PSD 2008). It is a solid at room temperature (Montgomery 1997). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.34.

Table 3.34 Physical-chemical data for β-hexachlorocyclohexane

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	4.71E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.72E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.84E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.87	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.23cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	290.83 g mol^{-1}	Recommended literature value
Vapour pressure	1.80E-05 Pa	Estimated by Grain-Watson method
Water solubility	0.2 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_6Cl_6$	
Boiling point	632.6 K	Estimated by MP correlation method
Critical point temperature	948.9 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	49,350 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.045 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	586.3 K	Recommended literature value
Physical state at room temperature	Solid	

3.35 γ-Hexachlorocyclohexane

γ-Hexachlorocyclohexane, lindane, γ-benzene hexachloride, or HCH (CAS No. 58-89-9) is **pesticide** and an **insecticide** (Montgomery 1997). HCH containing less than 99 per of the gamma **isomer** is banned from use in the UK (PSD 2008). It is a colourless crystalline solid at room temperature with a slightly musty odour (MERCK 2006, Montgomery 1997). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.35.

Table 3.35 Physical-chemical data for γ-hexachlorocyclohexane

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.1E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	4.78E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.84E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.67	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.07 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	290.83 g mol^{-1}	Recommended literature value
Vapour pressure	3.70E-03 Pa	Estimated by Grain-Watson method
Water solubility	7.3 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_6Cl_6$	
Boiling point	596.6 K	Recommended literature value
Critical point temperature	839.4 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	54,361 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.375 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	385.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.36 Indeno[123-cd]pyrene

Indeno[123-cd]pyrene (CAS No. 193-39-5) is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification (Montgomery 2007). It is a solid at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.36.

Table 3.36 Physical-chemical data for indeno[123-cd]pyrene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.05E-06	Estimated by Clapeyron relationship from the Henry's law constant at 20°C
Diffusion coefficient in air	4.17E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.51E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.97	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.94 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	276.33 g mol^{-1}	Recommended literature value
Vapour pressure	2.12E-09 Pa	Estimated by Grain-Watson method
Water solubility	2.0E-04 mg L^{-1} (20°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{22}H_{12}$	
Boiling point	809.2 K	Recommended literature value
Critical point temperature	1078.3 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	79,062 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.029 Pa $m^3\ mol^{-1}$ (20°C)	Recommended literature value
Melting point	435.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.37 Malathion

Malathion (CAS No. 121-75-5) is an **insecticide** for controlling chewing insects and spider mites on vegetables, fruits, field crops, gardens and forestry (Montgomery 1997). At **technical grade**, it is a yellow to dark brown liquid with a garlic or mercaptan-like odour (MERCK 2006, Montgomery 1997). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.37.

Table 3.37 Physical-chemical data for malathion

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	9.18E-07	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	4.12E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.27E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.90	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.59 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	330.36 g mol^{-1}	Recommended literature value
Vapour pressure	9.22E-04 Pa	Estimated by Grain-Watson method
Water solubility	141 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_{10}H_{19}O_6PS_2$	
Boiling point	653.6 K	Estimated by MP correlation method
Critical point temperature	980.4 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	62,730 J mol^{-1}	Estimated by Fishtine method
Henry's law constant	4.95E-04 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	276.1 K	Recommended literature value
Physical state at room temperature	Liquid	

3.38 Naphthalene

Naphthalene, mothballs, or tar camphor (CAS No. 91-20-3) is a chemical intermediate in the production of other compounds and is also used in the manufacture of dyes, explosives, mothballs, resins, celluloids, **pesticides**, detergents and wetting agents, synthetic tanning and preservatives (Montgomery 1997). It is a white, crystalline solid at room temperature with a strong aromatic odour associated with coal tar and mothballs (Montgomery 2007). It volatilises appreciably at room temperature (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.38.

Table 3.38 Physical-chemical data for naphthalene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.62E-03	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	6.52E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.16E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.34	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.81 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	128.17 g mol^{-1}	Recommended literature value
Vapour pressure	2.31 Pa	Estimated by Grain-Watson method
Water solubility	19 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_{10}H_8$	
Boiling point	491.1 K	Recommended literature value
Critical point temperature	748.4 K	Recommended literature value
Enthalpy of vaporisation at boiling point	43,200 J mol^{-1}	Recommended literature value
Henry's law constant	43 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	353.4 K	Recommended literature value
Physical state at room temperature	Solid	

3.39 Pentachlorobenzene

Pentachlorobenzene (CAS No. 608-93-5) is a contaminant in **dielectric fluids** and may be an undesired byproduct in the manufacture of hexachlorobenzene and chlorinated **solvents** including trichloroethene and 1,2-dichloroethane (Montgomery 2007). It is a solid at room temperature forming white needle shaped crystals (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.39.

Table 3.39 Physical-chemical data for pentachlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.30E-03	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.34E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.31E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.03	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.17 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	250.34 g mol^{-1}	Recommended literature value
Vapour pressure	6.33E-02 Pa	Estimated by Grain-Watson method
Water solubility	0.5 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_6HCl_5	
Boiling point	550.2 K	Recommended literature value
Critical point temperature	791.4 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	50,937 J mol^{-1}	Estimated by Klein method
Henry's law constant	85 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	359.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.40 Pentachlorophenol

Pentachlorophenol or PCP (CAS No. 87-86-5) is used as a **pesticide** and in the manufacture of other pesticides, and as wood preservative (Montgomery 2007). **Technical grades** may contain a wide range of impurities including hexachlorobenzene, PCBs, and other chlorinated phenols (Montgomery 2007). It is a solid at room temperature forming white flakes or needle-shaped crystals with a phenolic odour (Montgomery 2007). It is a weak acid (pK_a around five) with more than 99 per cent ionised in solution at pH 7 (Mackay *et al*. 2006, Montgomery 2007). The recommended physical-chemical data for the non-ionised compound for the derivation of Soil Guideline Values is shown in Table 3.40.

Table 3.40 Physical-chemical data for pentachlorophenol

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	5.55E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.17E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.21E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.07	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.97 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	266.34 g mol^{-1}	Recommended literature value
Vapour pressure	2.43E-04 Pa	Estimated by Grain-Watson method
Water solubility	14 mg L^{-1} (20°C)	Recommended literature value
Other useful data		
Chemical formula	C_6Cl_5OH	
Boiling point	583.2 K	Recommended literature value
Critical point temperature	814.7 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	59,678 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.079 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	447.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.41 Phenol

Phenol (CAS No. 108-95-2) is used as an antiseptic and disinfectant, and in the manufacture of pharmaceuticals, dyes, resins, and **polymers** (Montgomery 2007). It is also used as an industrial **solvent** for lubricating oils and in the manufacture of organic acids and phenols (Montgomery 2007). It is a colourless to white crystalline solid at room temperature with an acrid or sweet, tar-like odour (MERCK 2006, Montgomery 2007). It is a weak acid (pK_a around 10) with less than one per cent ionised in solution at pH 7 (Mackay *et al*. 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.41.

Table 3.41 Physical-chemical data for phenol

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.35E-06	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	7.90E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	6.36E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	1.48	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.92 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	94.11 g mol^{-1}	Recommended literature value
Vapour pressure	11.5 Pa	Estimated by Grain-Watson method
Water solubility	84,100 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_6H_5OH	
Boiling point	455.0 K	Recommended literature value
Critical point temperature	694.2 K	Recommended literature value
Enthalpy of vaporisation at boiling point	45,690 J mol^{-1}	Recommended literature value
Henry's law constant	0.065 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	314.0 K	Recommended literature value
Physical state at room temperature	Solid	

3.42 2-Propanone

2-Propanone, acetone or dimethyl ketone (CAS No. 67-64-1) is widely used in the production of other chemicals including acetic acid and chloroform, and as a general **solvent** in automotive engineering, paints, resins, surface coatings, varnishes and lacquers, paint and nail polish remover, and in the manufacture of rayon, photographic film, explosives, sealants and adhesives, pharmaceuticals and lubricating oils (MERCK 2006, Montgomery 1997). It is a clear, colourless and highly flammable liquid at room temperature with a sweet, fragrant odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.42.

Table 3.42 Physical-chemical data for 2-propanone

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.11E-04	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	1.03E-05 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	7.74E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	-0.24	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	0.90 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	58.08 g mol^{-1}	Recommended literature value
Vapour pressure	16,300 Pa	Estimated by Grain-Watson method
Water solubility	441,000 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_3H_6O	
Boiling point	329.3 K	Recommended literature value
Critical point temperature	508.1 K	Recommended literature value
Enthalpy of vaporisation at boiling point	29,100 J mol^{-1}	Recommended literature value
Henry's law constant	3.76 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	178.5 K	Recommended literature value
Physical state at room temperature	Liquid	

3.43 Pyrene

Pyrene or benzo[def]phenanthrene (CAS No. 129-00-0) is a polycyclic aromatic hydrocarbon formed as a byproduct of combustion processes including coal gasification (Montgomery 2007). It is a colourless to yellow solid at room temperature, the discolouration resulting from the presence of tetracene as an impurity (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.43.

Table 3.43 Physical-chemical data for pyrene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	5.64E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.01E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.15E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.08	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.21 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	202.25 g mol^{-1}	Recommended literature value
Vapour pressure	1.53E-05 Pa	Estimated by Grain-Watson method
Water solubility	0.13 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{16}H_{10}$	
Boiling point	677.2 K	Recommended literature value
Critical point temperature	951.1 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	62,675 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.920 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	423.8 K	Recommended literature value
Physical state at room temperature	Solid	

3.44 1,2,3,4-Tetrachlorobenzene

1,2,3,4-Tetrachlorobenzene (CAS No. 634-66-2) is used as a **dielectric fluid** and in organic synthesis (Montgomery 2007). It is a white crystalline solid at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.44.

Table 3.44 Physical-chemical data for 1,2,3,4-tetrachlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.58E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.69E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.59E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.54	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.78 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	215.89 g mol^{-1}	Recommended literature value
Vapour pressure	0.597 Pa	Estimated by Grain-Watson method
Water solubility	7.8 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_2Cl_4$	
Boiling point	527.2 K	Recommended literature value
Critical point temperature	771.8 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	48,250 J mol^{-1}	Estimated by Klein method
Henry's law constant	144 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	320.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.45 1,2,3,5-Tetrachlorobenzene

1,2,3,5-Tetrachlorobenzene (CAS No. 634-90-2) is used in organic synthesis (Montgomery 2007). It is a solid at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.45.

Table 3.45 Physical-chemical data for 1,2,3,5-tetrachlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.61E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.71E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.59E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.58	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.81 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	215.89 g mol^{-1}	Recommended literature value
Vapour pressure	0.753 Pa	Estimated by Grain-Watson method
Water solubility	3.5 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_2Cl_4$	
Boiling point	519.2 K	Recommended literature value
Critical point temperature	760.1 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	47,516 J mol^{-1}	Estimated by Klein method
Henry's law constant	588 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	327.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.46 1,2,4,5-Tetrachlorobenzene

1,2,4,5-Tetrachlorobenzene (CAS No. 95-94-3) is used in the manufacture of **insecticides** and in electrical insulation (Montgomery 2007). It is a white crystalline solid at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.46.

Table 3.46 Physical-chemical data for 1,2,4,5-tetrachlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.38E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.72E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.59E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.51	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.75 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	215.89 g mol^{-1}	Recommended literature value
Vapour pressure	9.04E-02 Pa	Estimated by Grain-Watson method
Water solubility	0.6 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_2Cl_4$	
Boiling point	517.7 K	Recommended literature value
Critical point temperature	757.9 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	47,379 J mol^{-1}	Estimated by Klein method
Henry's law constant	122 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	412.7 K	Recommended literature value
Physical state at room temperature	Solid	

3.47 1,1,1,2-Tetrachloroethane

1,1,1,2-Tetrachloroethane (CAS No. 630-20-6) is a chemical intermediate in the manufacture of trichloroethene and tetrachloroethene and occurs as an impurity in these widely used chemicals (IARC 1999). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.47.

Table 3.47 Physical-chemical data for 1,1,1,2-tetrachloroethane

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	4.80E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	6.90E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.43E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.03	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.55 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	167.85 g mol^{-1}	Recommended literature value
Vapour pressure	748 Pa	Estimated by Grain-Watson method
Water solubility	1,110 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_2H_2Cl_4$	
Boiling point	403.4 K	Recommended literature value
Critical point temperature	623.2 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	34,780 J mol^{-1}	Recommended literature value
Henry's law constant	245 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	203.0 K	Recommended literature value
Physical state at room temperature	Liquid	

3.48 1,1,2,2-Tetrachloroethane

1,1,2,2-Tetrachloroethane (CAS No. 79-34-5) was withdrawn from UK use as a **pesticide** in 1969 due to its acute and chronic toxicity to humans (PSD 2008). It is also used as an industrial **solvent** for chlorinated rubber, oils and fats, and metal degreasing, and also in the manufacture of paint, varnish, rust remover, and 1,1-dichloroethene (Montgomery 2007). It is a colourless to pale yellow, non-flammable liquid at room temperature with a sweet, chloroform-like odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.48.

Table 3.48 Physical-chemical data for 1,1,2,2-tetrachloroethane

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	7.08E-03	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	6.84E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.43E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.39	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.04 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	167.85 g mol^{-1}	Recommended literature value
Vapour pressure	291 Pa	Estimated by Grain-Watson method
Water solubility	2,930 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_2H_2Cl_4$	
Boiling point	419.7 K	Recommended literature value
Critical point temperature	661.2 K	Recommended literature value
Enthalpy of vaporisation at boiling point	37,640 J mol^{-1}	Recommended literature value
Henry's law constant	46.1 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	230.8 K	Recommended literature value
Physical state at room temperature	Liquid	

3.49 Tetrachloroethene

Tetrachloroethene, tetrachloroethylene, perchloroethene, perchloroethylene, PCE or ‘Perc’ (CAS No. 127-18-4) is used in dry cleaning, degreasing and drying metals, heat-exchange and insulation fluids in electrical transformers, **vermifuge**, and in the manufacturing of printing inks, paint removers, and fluorocarbons (MERCK 2006, Montgomery 2007). It is also a general **solvent** for waxes, greases, fats, oils and gums (Montgomery 2007). It is a clear, colourless and non-flammable liquid at room temperature with sweet ethereal or chloroform-like odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.49.

Table 3.49 Physical-chemical data for tetrachloroethene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.16E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.10E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.61E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.88	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.43 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	165.83 g mol^{-1}	Recommended literature value
Vapour pressure	1,010 Pa	Estimated by Grain-Watson method
Water solubility	225 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_2Cl_4	
Boiling point	394.5 K	Recommended literature value
Critical point temperature	620.2 K	Recommended literature value
Enthalpy of vaporisation at boiling point	34,680 J mol^{-1}	Recommended literature value
Henry’s law constant	1,730 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	250.9 K	Recommended literature value
Physical state at room temperature	Liquid	

3.50 Tetrachloromethane

Tetrachloromethane or carbon tetrachloride (CAS No. 56-23-5) is used in the preparation of refrigerants, aerosols, and propellants, as a metal degreaser and a **solvent** for fats, oils and rubber, and in the manufacture of veterinary medicines (Montgomery 2007). It was formerly used as a dry cleaning agent, in fire extinguishers, and as a grain **fumigant** (MERCK 2006). It is a clear, colourless, non-flammable liquid with a strong sweet ether-like odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.50.

Table 3.50 Physical-chemical data for tetrachloromethane

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	5.82E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.69E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	6.03E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.83	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.39 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	153.82 g mol^{-1}	Recommended literature value
Vapour pressure	7,530 Pa	Estimated by Grain-Watson method
Water solubility	846 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	CCl_4	
Boiling point	350.0 K	Recommended literature value
Critical point temperature	556.6 K	Recommended literature value
Enthalpy of vaporisation at boiling point	29,820 J mol^{-1}	Recommended literature value
Henry's law constant	2,990 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	250.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.51 2,3,4,6-Tetrachlorophenol

2,3,4,6-Tetrachlorophenol (CAS No. 58-90-2) is used as a **fungicide** for treating timber against fungi and surface mould, and as an additive to inhibit microbial growth in a wide array of products such as adhesives, oils, textiles, and pharmaceutical products (IPCS 1989). At **technical grade**, it is a solid at room temperature with a strong and pungent medicinal-like odour and often contains other chlorophenols as impurities including pentachlorophenol (IPCS 1989). It is also a weak acid (pK_a around 5.5) with more than 95 per cent ionised in solution at pH 7 (Mackay *et al*. 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.51.

Table 3.51 Physical-chemical data for 2,3,4,6-tetrachlorophenol

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.96E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.54E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.49E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.42	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.60 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	231.89 g mol^{-1}	Recommended literature value
Vapour pressure	0.219 Pa	Estimated by Grain-Watson method
Water solubility	183 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_6HCl_4OH	
Boiling point	542.3 K	Estimated by MP correlation method
Critical point temperature	813.5 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	48,392 J mol^{-1}	Estimated by Klein method
Henry's law constant	0.355 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	343.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.52 Tetraethyl lead

Tetraethyl lead or tetraethyl plumbane (CAS No. 78-00-2) was used as an **anti-knock** additive in petrol (MERCK 2006). It is a colourless, flammable liquid at room temperature (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.52.

Table 3.52 Physical-chemical data for tetraethyl lead

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	6.20E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.51E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.37E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.88	Estimated by KOWWIN method
Log (Organic carbon-water partition coefficient) (K_{oc})	3.56 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	323.44 g mol^{-1}	Recommended literature value
Vapour pressure	1.45 Pa	Estimated by Grain-Watson method
Water solubility	3.2 mg L^{-1} (25°C)	Estimated by WSKOWIN method
Other useful data		
Chemical formula	$C_8H_{20}Pb$	
Boiling point	473.2 K	Recommended literature value
Critical point temperature	709.8 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	56,600 J mol^{-1}	Recommended literature value
Henry's law constant	665 Pa m^3 mol^{-1} (25°C)	Estimated by direct calculation at 25°C
Melting point	142.9 K	Recommended literature value
Physical state at room temperature	Liquid	

3.53 Toluene

Toluene, methylbenzene, or methyl-benzol (CAS No. 108-88-3) is used widely in the manufacture of medicines, detergents, dyes, perfumes, other substituted aromatic compounds, as a **solvent** for paints, gums, resins, rubber, oils, plastic toys, and as additive to aviation fuel and other high octane fuels (Montgomery 2007). It is a colourless, clear, flammable liquid at room temperature with a pleasant, sweet or paint-like odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.53.

Table 3.53 Physical-chemical data for toluene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.15E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.78E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.88E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.73	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.31 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	92.14 g mol^{-1}	Recommended literature value
Vapour pressure	1,730 Pa	Estimated by Grain-Watson method
Water solubility	590 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_6H_5CH_3$	
Boiling point	383.8 K	Recommended literature value
Critical point temperature	591.8 K	Recommended literature value
Enthalpy of vaporisation at boiling point	33,180 J mol^{-1}	Recommended literature value
Henry's law constant	660 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	178.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.54 Tributyl tin oxide

Tributyl tin oxide, TBTO, or hexabutyldistannoxane (CAS No. 56-35-9) is an effective **biocide** preservative for wood, cotton textiles, paper, and paints for residential homes (IPCS 1999). It is an **antifouling agent** in numerous formulations of marine paints as an organometallic copolymer (IPCS 1999). It is a low volatile, flammable liquid at room temperature (IPCS 1999). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.54.

Table 3.54 Physical-chemical data for tributyl tin oxide

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	4.24E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	3.25E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	2.49E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.05	Estimated by KOWWIN method
Log (Organic carbon-water partition coefficient) (K_{oc})	3.13 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	596.11 g mol^{-1}	Recommended literature value
Vapour pressure	8.56E-04 Pa	Estimated by Grain-Watson method
Water solubility	5.1 mg L^{-1} (25°C)	Estimated by WSKOWIN method
Other useful data		
Chemical formula	$C_{24}H_{54}OSn_2$	
Boiling point	654.9 K	Estimated by Banks method
Critical point temperature	982.4 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	62,867 J mol^{-1}	Estimated by Fishtine method
Henry's law constant	6.01E-01 Pa m^3 mol^{-1} (25°C)	Estimated by direct calculation at 25°C
Melting point	228.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.55 1,2,3-Trichlorobenzene

1,2,3-Trichlorobenzene or 1,2,3-TCB (CAS No. 87-61-6) is used in the synthesis of other organic compounds and in other countries as a control for termites (Montgomery 2007). It occurs as white crystals or platelets at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.55.

Table 3.55 Physical-chemical data for 1,2,3-trichlorobenzene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.07E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	6.16E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.94E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.09	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.41 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	181.45 g mol^{-1}	Recommended literature value
Vapour pressure	3.5 Pa	Estimated by Grain-Watson method
Water solubility	21 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_3Cl_3$	
Boiling point	491.7 K	Recommended literature value
Critical point temperature	733.5 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	44,523 J mol^{-1}	Estimated by Klein method
Henry's law constant	242 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	324.5 K	Recommended literature value
Physical state at room temperature	Solid	

3.56 1,2,4-Trichlorobenzene

1,2,4-Trichlorobenzene, 1,2,4-TCB, or *unsym*-trichlorobenzene (CAS No. 120-82-1) is used as a **solvent** in the manufacture of organic chemicals including dyes, dielectric fluids, synthetic transformer oils, lubricants, and **insecticides** (Montgomery 2007). It is a colourless liquid at room temperature with an odour similar to 1,2-dichlorobenzene (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.56.

Table 3.56 Physical-chemical data for 1,2,4-trichlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.65E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	6.17E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.94E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.03	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.36 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	181.45 g mol^{-1}	Recommended literature value
Vapour pressure	11.1 Pa	Estimated by Grain-Watson method
Water solubility	41.4 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_3Cl_3$	
Boiling point	486.7 K	Recommended literature value
Critical point temperature	730.7 K	Recommended literature value
Enthalpy of vaporisation at boiling point	43,464 J mol^{-1}	Estimated by Klein method
Henry's law constant	277 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	290.2 K	Recommended literature value
Physical state at room temperature	Liquid	

3.57 1,3,5-Trichlorobenzene

1,3,5-Trichlorobenzene or 1,3,5-TCB (CAS No. 108-70-3) is used in the synthesis of other organic compounds (Montgomery 2007). It is a crystalline solid at room temperature (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.57.

Table 3.57 Physical-chemical data for 1,3,5-trichlorobenzene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.44E-01	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	6.19E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.94E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	4.10	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.42 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	181.45 g mol^{-1}	Recommended literature value
Vapour pressure	4.41 Pa	Estimated by Grain-Watson method
Water solubility	6 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_3Cl_3$	
Boiling point	481.2 K	Recommended literature value
Critical point temperature	717.9 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	43,564 J mol^{-1}	Estimated by Klein method
Henry's law constant	1,100 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	336.0 K	Recommended literature value
Physical state at room temperature	Solid	

3.58 1,1,1-Trichloroethane

1,1,1-Trichloroethane, methyl chloroform, chlorothene, or 1,1,1-TCA (CAS No. 71-55-6) is used widely in the synthesis of other organic compounds, as a metal cleaner and degreaser, and in the manufacture of textiles, aerosol propellants, coatings and inks, adhesives and cutting oils, and as a **pesticide** (MERCK 2006, Montgomery 2007). It is a colourless, watery liquid at room temperature with a sweet, sharp or polish-like odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.58.

Table 3.58 Physical-chemical data for 1,1,1-trichloroethane

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.60E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.75E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.99E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.49	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.12 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	133.40 g mol^{-1}	Recommended literature value
Vapour pressure	8,250 Pa	Estimated by Grain-Watson method
Water solubility	1,300 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$C_2H_3Cl_3$	
Boiling point	347.2 K	Recommended literature value
Critical point temperature	545.0 K	Recommended literature value
Enthalpy of vaporisation at boiling point	29,860 J mol^{-1}	Recommended literature value
Henry's law constant	1,710 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	243.1 K	Recommended literature value
Physical state at room temperature	Liquid	

3.59 Trichloroethene

Trichloroethene, trichloroethylene, TCE or 'Trike' (CAS No. 79-01-6) is used as a dry cleaning agent, in the degreasing and drying of metals and electronics, as a **solvent** for oils, waxes, fats, cellulose esters and ethers, paints, adhesives, and the removal of caffeine from coffee (Montgomery 2007). It is also used as a refrigerant, **fumigant**, anesthetic, and in the synthesis of organic chemicals including hydrofluorocarbons (Montgomery 2007). It is a clear, colourless, non-flammable, watery liquid at room temperature with a chloroform-like odour (MERCK 2006, Montgomery 2007). It slowly decomposes to hydrochloric acid in the presence of moisture and light (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.59.

Table 3.59 Physical-chemical data for trichloroethene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.87E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.91E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	6.23E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.53	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.15 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	131.39 g mol^{-1}	Recommended literature value
Vapour pressure	4,580 Pa	Estimated by Grain-Watson method
Water solubility	1,370 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_2HCl_3	
Boiling point	360.4 K	Recommended literature value
Critical point temperature	544.2 K	Recommended literature value
Enthalpy of vaporisation at boiling point	31,400 J mol^{-1}	Recommended literature value
Henry's law constant	1,030 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	188.5K	Recommended literature value
Physical state at room temperature	Liquid	

3.60 Trichloromethane

Trichloromethane or chloroform (CAS No. 67-66-3) is used in the manufacture of fluorocarbon refrigerants, plastics, propellants and fire extinguishers, and as a soil **fumigant**, **insecticide** and **solvent** for cleaning electronic circuit boards (MERCK 2006, Montgomery 2007). It is a colourless, clear, non-flammable, volatile and heavy liquid at room temperature with a strong, sweet, antiseptic or ether-like odour (MERCK 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.60.

Table 3.60 Physical-chemical data for trichloromethane

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	7.65E-02	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	8.60E-06 m^2 s^{-1}	Estimated by Wilke and Lee method
Diffusion coefficient in water	6.80E-10 m^2 s^{-1}	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	1.97	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	1.70 cm^3 g^{-1}	Estimated by linear regression from log K_{ow}
Molecular weight	119.38 g mol^{-1}	Recommended literature value
Vapour pressure	13,500 Pa	Estimated by Grain-Watson method
Water solubility	8,950 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	$CHCl_3$	
Boiling point	334.3 K	Recommended literature value
Critical point temperature	536.4 K	Recommended literature value
Enthalpy of vaporisation at boiling point	29,240 J mol^{-1}	Recommended literature value
Henry's law constant	430 Pa m^3 mol^{-1} (25°C)	Recommended literature value
Melting point	209.7 K	Recommended literature value
Physical state at room temperature	Liquid	

3.61 2,4,6-Trichlorophenol

2,4,6-Trichlorophenol (CAS No. 88-06-2) is used in the manufacture of **fungicides**, **bactericides**, antiseptics, wood and glue preservatives, and as an intermediate in the formation of higher chlorinated phenols (MERCK 2006, Montgomery 2007). It is also used as a defoliant, disinfectant, and in the synthesis of other organic chemicals (Montgomery 2007). It forms either colourless needle-shaped crystals or a yellow crystalline solid at room temperature with a strong phenolic odour (Montgomery 2007). It is also a weak acid (pK_a around six) with more than 90 per cent ionised in solution at pH 7 (Mackay *et al*. 2006, Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.61.

Table 3.61 Physical-chemical data for 2,4,6-trichlorophenol

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	8.82E-07	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.94E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.81E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.69	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	3.18 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	197.45 g mol^{-1}	Recommended literature value
Vapour pressure	0.174 Pa	Estimated by Grain-Watson method
Water solubility	434 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_6H_2Cl_3OH$	
Boiling point	519.2 K	Recommended literature value
Critical point temperature	749.1 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	52,408 J mol^{-1}	Estimated by Klein method
Henry's law constant	9.19E-03 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	342.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.62 α,α,α-Trichlorotoluene

α,α,α-Trichlorotoluene, benzotrichloride, or (trichloromethyl)-benzene (CAS No. 98-07-7) is used in dye manufacture and the synthesis of other organic chemicals (MERCK 2006). It is a colourless, oily liquid at room temperature with a pungent odour (MERCK 2006). It is unstable and hydrolyses in the presence of moisture to form benzoic and hydrochloric acids (MERCK 2006). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.62.

Table 3.62 Physical-chemical data for trichlorotoluene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	3.20E-03	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	5.79E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	4.57E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	2.92	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.47 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	195.47 g mol^{-1}	Recommended literature value
Vapour pressure	11 Pa	Estimated by Grain-Watson method
Water solubility	370 mg L^{-1} (25°C)	Estimated by WSKOWIN method
Other useful data		
Chemical formula	$C_7H_5Cl_3$	
Boiling point	494.2 K	Recommended literature value
Critical point temperature	737.3 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	43,181 J mol^{-1}	Estimated by Klein method
Henry's law constant	24 Pa $m^3\ mol^{-1}$ (25°C)	Estimated by direct calculation at 25°C
Melting point	268.7 K	Recommended literature value
Physical state at room temperature	Liquid	

3.63 Trifluralin

Trifluralin or 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine (CAS No. 1582-09-8) is a pre-emergence **herbicide** used to control annual grasses and broad-leaved weeds in fruit and vegetable crops (MERCK 2006, Montgomery 2007). It is a solid at room temperature with yellow to reddish-orange crystals (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.63.

Table 3.63 Physical-chemical data for trifluralin

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	2.87E-04	Estimated by Clapeyron relationship from the Henry's law constant at 23°C
Diffusion coefficient in air	4.29E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	3.42E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	5.23	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	4.19 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	335.28 g mol^{-1}	Recommended literature value
Vapour pressure	4.46E-05 Pa	Estimated by Grain-Watson method
Water solubility	1 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	$C_{13}H_{16}F_3N_3O_4$	
Boiling point	635.2 K	Recommended literature value
Critical point temperature	795.5 K	Estimated by Lydersen method
Enthalpy of vaporisation at boiling point	71,926 J mol^{-1}	Estimated by Klein method
Henry's law constant	5.91 Pa $m^3 mol^{-1}$ (23°C)	Recommended literature value
Melting point	322.2 K	Recommended literature value
Physical state at room temperature	Solid	

3.64 m-Xylene

m-Xylene, 1,3-xylene or 1,3-dimethylbenzene (CAS No. 108-38-3) is used widely as a **solvent** and in the manufacture of dyes, **insecticides** and aviation fuel (Montgomery 2007). It is a clear, colourless, watery liquid at room temperature with a sweet, aromatic odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.64.

Table 3.64 Physical-chemical data for m-Xylene

Chemical Property		**Comments**
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.12E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.03E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.31E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.20	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.69 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	106.17 g mol^{-1}	Recommended literature value
Vapour pressure	495 Pa	Estimated by Grain-Watson method
Water solubility	200 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_8H_{10}	
Boiling point	412.5 K	Recommended literature value
Critical point temperature	617.0 K	Recommended literature value
Enthalpy of vaporisation at boiling point	35,660 J mol^{-1}	Recommended literature value
Henry's law constant	730 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	225.4 K	Recommended literature value
Physical state at room temperature	Liquid	

3.65 o-Xylene

o-Xylene, 1,2-xylene or 1,2-dimethylbenzene (CAS No. 95-47-6) is used widely as a **solvent** and in the manufacture of lacquers, enamels, rubber cements, dyes, pharmaceuticals, **insecticides** and motor fuels (Montgomery 2007). It is a clear, colourless, watery liquid at room temperature with an aromatic odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.65.

Table 3.65 Physical-chemical data for o-xylene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	9.20E-02	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	7.01E-06 $m^2 s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.31E-10 $m^2 s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.12	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.63 $cm^3 g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	106.17 g mol^{-1}	Recommended literature value
Vapour pressure	386 Pa	Estimated by Grain-Watson method
Water solubility	173 mg L^{-1} (25°C)	Recommended literature value
Other useful data		
Chemical formula	C_8H_{10}	
Boiling point	417.6 K	Recommended literature value
Critical point temperature	630.3 K	Recommended literature value
Enthalpy of vaporisation at boiling point	36,240 J mol^{-1}	Recommended literature value
Henry's law constant	551 Pa $m^3 mol^{-1}$ (25°C)	Recommended literature value
Melting point	248.0 K	Recommended literature value
Physical state at room temperature	Liquid	

3.66 p-Xylene

p-Xylene, 1,4-xylene or 1,4-dimethylbenzene (CAS No. 106-42-3) is used widely as a **solvent** and in the manufacture of polyester resins and fibres, pharmaceuticals, **insecticides** and petrol (Montgomery 2007). It is a clear, colourless, watery liquid at room temperature with a sweet odour (Montgomery 2007). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.64.

Table 3.66 Physical-chemical data for p-xylene

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient (K_{aw})	1.07E-01	Estimated by direct calculation from water solubility and vapour pressure at 10°C
Diffusion coefficient in air	7.04E-06 $m^2\ s^{-1}$	Estimated by Wilke and Lee method
Diffusion coefficient in water	5.31E-10 $m^2\ s^{-1}$	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) (K_{ow})	3.15	Recommended literature value
Log (Organic carbon-water partition coefficient) (K_{oc})	2.65 $cm^3\ g^{-1}$	Estimated by linear regression from log K_{ow}
Molecular weight	106.17 g mol^{-1}	Recommended literature value
Vapour pressure	475 Pa	Estimated by Grain-Watson method
Water solubility	200 mg L^{-1}	Recommended literature value
Other useful data		
Chemical formula	C_8H_{10}	
Boiling point	411.5 K	Recommended literature value
Critical point temperature	616.2 K	Recommended literature value
Enthalpy of vaporisation at boiling point	35,670 J mol^{-1}	Recommended literature value
Henry's law constant	669 Pa $m^3\ mol^{-1}$ (25°C)	Recommended literature value
Melting point	286.4 K	Recommended literature value
Physical state at room temperature	Liquid	

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List of abbreviations

AQUAFAC	Aqueous Functional Group Activity Coefficients
BTEX	Benzene, toluene, ethylbenzene and xylene
CAS	Chemical Abstracts Service
CLEA	Contaminated Land Exposure Assessment model
CLR	Contaminated Land Research
CODATA	Committee on Data for Science and Technology for international use
dec	decomposes on heating
Defra	Department for Environment, Food and Rural Affairs
DDT	Dichlorodiphenyltrichloroethane
ECB	European Chemicals Bureau
EPI	Estimation Programs Interface suite
EU	European Union
FSG	Fuller, Schettler and Giddings method
HCH	Hexachlorocyclohexane
HLC	Henry’s law constant
HPA	Health Protection Agency
IARC	International Agency for Research on Cancer
IPCS	International Programme on Chemical Safety (World Health Organisation)
IUPAC	International Union for Pure and Applied Chemistry
K_{aw}	Air-water partition coefficient
K_{oc}	Organic carbon-water partition coefficient

K_{ow}	Octanol-water partition coefficient
m-	meta position substitution on a benzene ring
MOL	File extension of the MDL Molfile chemical file format
MP	Melting Point
NA	Not Available
NIST	National Institute of Standards and Technology
o-	ortho position substitution on a benzene ring
p-	para position substitution on a benzene ring
low P	Boiling point measured at air pressure less than one atmosphere
PAH	Polycyclic aromatic hydrocarbons
PC	Personal Computer
PCB	Polychlorinated biphenyls
PSD	Pesticide Safety Directorate
QSAR	Quantitative Structure Activity Relationships
SGV	Soil Guideline Value
SI	International System of Units
SMILES	Simplified Molecular Input Line Entry Specification
SOM	Soil organic matter
sub	sublimes on heating
TBTO	Tributyl tin oxide
TPH	Total Petroleum Hydrocarbons
TPHCWG	Total Petroleum Hydrocarbons Criteria Working Group
UK	United Kingdom

USEPA	United States Environmental Protection Agency
VOC	Volatile organic compounds
WL	Wilke and Lee method

Glossary

Advection	The movement of a fluid (liquid, gas) as part of the bulk movement of air and water, under the influence of differences in pressure, temperature and density between locations.
Antiknock agent	A substance added to petrol to reduce engine knocking caused by too rapid fuel ignition.
Antifouling agent	A substance applied to underwater surfaces, such as the hull of ships, to prevent the accumulation of microorganisms, plants, algae and animals.
Bactericide	A substance that kills bacteria.
Biocide	A substance that kills living organisms, usually selectively.
Commercial grade	Chemicals produced in bulk for general commercial use, usually containing impurities from the production process.
Constant of proportionality	The ratio between two variables that change in proportion to one another.
Dielectric fluid	A fluid that does not conduct an electric current.
Dermal	Of or pertaining to the skin.
Diffusion	Random movement of molecules due to their inherent kinetic energy.
Dipole-dipole interactions	The attractive and repulsive interactions between molecules carrying both a positive and negative charge due to the uneven distribution of electrons between atoms forming a covalent bond.
Dipole moment	A measure of the polarity of a molecule due to the non-uniform distribution of electrons.
Empirical models	A model based only on experimental observation that is used to establish plausible relationships between parameters.
Endothermic	A process or reaction that absorbs energy in the form of heat.
Equilibrium	The state in which there is no net change, for example, in concentrations or chemical activities, over time, with the rate of the forward process being equal to that of the reverse process.
Exposure	Contact between a chemical and the external surfaces of the human body. Quantitatively, it is the amount of a chemical that is available for intake by a target receptor/population. Exposure may be quantified as the dose or the concentration of the chemical in the medium (for example, air, water, food) integrated over the duration of exposure, expressed in terms of mass of substance per kg of soil, cubic metre of air, or litre of water.
Fick’s law	A law relating the rate of diffusion of a substance in a given direction to the gradient of its concentration.
Fugacity ratio	The ratio of the solid and liquid vapour pressures of a chemical, used to estimate properties of the chemical in the liquid state at ambient temperatues when it has

	a melting point above ambient temperature.
Fumigant	A substance used in its gaseous state as a pesticide or disinfectant.
Functional group	An atom or group of atoms in a molecule that undergo characteristic chemical reactions and influence chemical properties of the compound, for example, hydroxyl (-OH) and amino ($-NH_2$) groups.
Germicide	A substance used to kill pathogenic microorganisms.
Generic Assessment Criteria	Criteria derived using largely generic assumptions about the characteristics and behaviour of sources, pathways and receptors. These assumptions will be conservative in a defined range of conditions.
Generic quantitative risk assessment	The purpose of generic quantitative risk assessment is to establish whether generic assessment criteria and assumptions are appropriate for assessing the risks, and, if so, to apply them to establish whether there are actual or potential unacceptable risks.
Henry's law constant	The constant of proportionality between water solubility and the partial pressure of the gas phase.
Herbicide	A substance used to kill or inhibit the growth of plants or weeds.
Hydrogen bonding	A strong dipole-dipole attraction between an electronegative (electron-attracting) atom and a hydrogen atom attached to a second, relatively electronegative atom, particularly oxygen, nitrogen and fluorine, and to a lesser extent phosphorus, sulphur and chlorine.
Hydrophilic	Literally 'water-loving'. Describes the character of a molecule which has an affinity for water and therefore high aqueous solubility.
Hydrophobic	Literally 'water-hating', hydrophobic describes compounds with a low aqueous solubility that are more fat soluble.
Ideal gas law	The equation of state that defines an ideal gas. The equation is $pV=RT$, where p is pressure, V is molar volume, T is temperature and R is the molar gas constant.
Insecticide	A substance used to kill insects at any developmental stage.
Ionisation	The loss or gain of electrons of an atom or molecule, producing a net electric charge.
Lipophilic	The term used to describe compounds with a high solubility in fat and low aqueous solubility. Such substances will have a high octanol-water partition coefficient (K_{ow}).
Mechanistic model	A model that establishes a plausible relationship between parameters based on theoretical understanding of the processes and mechanisms that give rise to the system being investigated.
Molar volume	The volume occupied by one mole of a substance at a specified temperature and pressure.
Partial pressure	The pressure that a component, X, of a gas mixture would exhibit if X alone occupied the total volume of the mixture, at the temperature of the mixture.

Pesticide	A general term used to describe a substance that kills pests, including plants, mammals or insects.
Polar chemical	A substance consisting of molecules with an unequal distribution of electrons between atoms, resulting in negatively and positively charged portions of the molecule.
Polymer	A substance consisting of high molecular weight molecules which have a structure comprising multiple repetitions of low molecular weight units.
Polymerise	Undergo a chemical reaction to form a polymer.
Proportionality constant	See ‘constant of proportionality’
Quantitative Structure Activity Realtionship	Estimation methods developed and used to predict certain effects or properties of chemical substances that are primarily based on the structure of the substance. They have been developed on the basis of experimental data on model substances.
Site-specific assessment criteria	Values for concentrations of contaminants that have been derived using detailed site-specific information on the characteristics and behaviour of contaminants, pathways and receptors, and that correspond to relevant criteria in relation to harm or pollution for deciding whether there is an unacceptable risk.
Soil Guideline Values	Non-statutory and scientifically based generic assessment criteria for assessing the risk to human health from chronic exposures to chemicals in soil.
Solvent	Typically a liquid in which a solid, liquid or gas (solute) is dissolved to form a solution.
Sorption	Describes either an absorptive or adsorptive process. The term may be used where the exact process is not known.
Stereoisomer	A molecule with the same atoms bonded together as another molecule but in a different spatial arrangement.
Sublime	To change directly from the solid to gas phase with no intermediate liquid phase.
Technical grade	Form of a chemical containing impurities from the production process.
Thermodynamic properties	Values that define the potential of a chemical substance to undergo reactions or phase changes, and depend upon the energy required to make or break bonds.
Triazine ring	A ring structure composed of three carbon and three nitrogen atoms. Three isomers of the structure are distinguished from one another by the position of their N atoms.
Van der Waals forces	The weak attractive and repulsive forces occurring between molecules due to temporary polarisation of molecules.
Walden’s rule	The entropy of fusion of a chemical (the enthalpy of fusion divided by the melting point temperature) is typically 56.5.

Appendix A

Compilation of physical-chemical data from authoritative sources

Table A1: Boiling point at ambient pressure (K)

Chemical	Chemical Group	Boiling point at ambient pressure (K)		Consensus
		Review	Recommended	
Aldrin	Pesticide	low P [c, e, f]	none	
Atrazine	Pesticide	dec [f]	none	
Azinphos-methyl	Pesticide	dec [c, d, f]	none	
Benzene	BTEX	353.2 [b, c, e], 353.3 [a, d, g, h]	353.2	High
Benzo[*a*]anthracene	PAH	692 [e], 710.8 [g], 711.2 [b, c]	711.2	Medium
Benzo[*b*]fluoranthene	PAH	754.2 [c]	754.2	Very Low
Benzo[*k*]fluoranthene	PAH	753.2 [b, c, g], 754.2 [e]	753.2	Medium
Benzo[*ghi*]perylene	PAH	798.2 [c, e]	798.2	Low
Benzo[*a*]pyrene	PAH	low P [d], 768.2 [c, e, g]	768.2	Low
Carbon disulphide		319.2 [b, c, g], 319.4 [f], 319.7 [a, d], 320.2 [e]	319.2	High
Chlorobenzene	Chlorobenzene	404.7 [d], 404.9 [b, c, e, g], 405.2 [a]	404.9	High
Chloroethene		259.2 [h], 259.4 [b, c, g], 259.8 [a, d, e]	259.4	High
2-Chlorophenol	Chlorophenol	447.9 [e], 448.1 [a, b, c, g], 448.2 [d]	448.1	High
α-Chlorotoluene	Chlorotoluene	452.0 [g], 452.2 [a, b, c, d, h], 452.5 [e]	452.2	High
2-Chlorotoluene	Chlorotoluene	432.1 [d, g], 432.2 [b, c], 432.5 [h]	432.2	Medium
Chrysene	PAH	721.2 [b, c, d, e, g]	721.2	High
p,*p*'-DDT	Pesticide	dec [f], 533.2 [c, e]	533.2	Low
o,*p*'-DDT	Pesticide	533.2 [c]	533.2	Very Low
Dibenz[*ah*]anthracene	PAH	797.2 [c, e, g]	797.2	Low
1,2-Dichlorobenzene	Chlorobenzene	453.2 [b, c], 453.3 [e], 453.5 [h], 453.7 [a, d, g]	453.7	High
1,3-Dichlorobenzene	Chlorobenzene	446.2 [a, b, c, d, g], 446.7 [e]	446.2	High
1,4-Dichlorobenzene	Chlorobenzene	447.0 [e], 447.2 [a, b, c, h], 447.3 [d, g]	447.2	High
1,2-Dichloroethane		356.4 [e], 356.6 [a], 356.7 [b, g], 357.0 [h], 358.5 [c]	356.7	Medium
2,4-Dichlorophenol	Chlorophenol	481.7 [h], 483.2 [b, c, d, g], 486.2 [e]	483.2	Medium
Dichlorvos	Pesticide	low P [a, b, d, e, f], 507.2 [c]	507.2	Very Low
Dieldrin	Pesticide	dec [e, f], 538 – 677 [c]	none	
Endosulfan (α form)	Pesticide	low P [b, c]	none	
Endosulfan (β form)	Pesticide	low P [b, c]	none	
Ethylbenzene	BTEX	409.3 [b, e, g], 409.4 [a, c, d, h]	409.4	High

Chemical	Chemical Group	Boiling point at ambient pressure (K)		Consensus
		Review	Recommended	
Fenitrothion	Pesticide	low P [b, c, d]	none	
Fluoranthene	PAH	657.2 [b, c, e]	657.2	Low
Hexachlorobenzene	Chlorobenzene	597.5 [a, f], 597.7 [d, e, g], 598.2 [b, c]	597.7	High
Hexchloro-1,3-butadiene		488.2 [a, b, c, d, e, g]	488.2	High
α-Hexachlorocyclohexane	Pesticide	561.2 [a, c, e, f]	561.2	Medium
β-Hexachlorocyclohexane	Pesticide	low P [b], sub [e, f]	none	
γ-Hexachlorocyclohexane	Pesticide	596.2 [c], 596.6 [a, b, e, f]	596.6	Medium
Indeno[*123-cd*]pyrene	PAH	809.2 [e]	809.2	Very Low
Malathion	Pesticide	dec [b, f], low P [a, b, c, d, e]	none	
Naphthalene	PAH	490.0 [g], 491.1 [a, b, c, d, e], 491.2 [h]	491.1	High
Pentachlorobenzene	Chlorobenzene	550.2 [b, c, e, f, g]	550.2	High
Pentachlorophenol	Chlorophenol	582.7 [a, d], 583.2 [b, c, e, f, g]	583.2	High
Phenol		454.9 [a], 455.0 [b, c, g], 455.2 [d, h], 456.2 [e]	455.0	High
2-Propanone		329.2 [b, c], 329.3 [e, g, h], 329.4 [a], 329.7 [d]	329.3	High
Pyrene	PAH	666.2 [e], 677.2 [b, c, d]	677.2	Medium
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	527.2 [b, c, e, g]	527.2	Medium
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	519.2 [b, c, e, g]	519.2	Medium
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	516.2 [g], 517.7 [b, c, e]	517.7	Medium
1,1,1,2-Tetrachloroethane		403.4 [b, c], 403.7 [a], 406.0 [g]	403.4	Medium
1,1,2,2-Tetrachloroethane		418.4 [b, c], 419.3 [e, g], 419.7 [a, d, h]	419.7	High
Tetrachloroethene		394.2 [a, d, g], 394.5 [b, c, e]	394.5	High
Tetrachloromethane		349.7 [a, f], 349.8 [g], 349.9 [d], 350.0 [b, c], 350.7 [e]	350.0	High
2,3,4,6-Tetrachlorophenol	Chlorophenol	low P [b]	none	
Tetraethyl lead		455.7 [g], 473.2 [b, d]	473.2	Low
Toluene	BTEX	383.8 [a, b, c, d, e, g, h]	383.8	Very High
Tributyl tin oxide (TBTO)		low P [b, g]	none	
1,2,3-Trichlorobenzene	Chlorobenzene	491.7 [b, c, e, g], 494.2 [d]	491.7	Medium
1,2,4-Trichlorobenzene	Chlorobenzene	486.2 [d], 485.4 [h], 486.6 [e], 486.7 [a, b, c, g]	486.7	High
1,3,5-Trichlorobenzene	Chlorobenzene	481.2 [a, b, c, e, g], 481.6 [d]	481.2	High
1,1,1-Trichloroethane		347.0 [e], 347.2 [b, c, g], 347.3 [a, d]	347.2	High
Trichloroethene		360.0 [h], 360.1 [d], 360.2 [a, g], 360.4 [b, c, e]	360.4	High
Trichloromethane		334.2 [e], 334.3 [b, c, g], 334.7 [d], 334.9 [a]	334.3	High
2,4,6-Trichlorophenol	Chlorophenol	519.2 [a, b, c, d, e, g]	519.2	Very High
α,α,α-Trichlorotoluene	Chlorotoluene	493.8 [g], 493.9 [h], 494.0 [a, d], 494.2 [b, c]	494.2	High
Trifluralin	Pesticide	low P [b, d, e, f], 635.2 [c]	635.2	Very Low

Chemical	Chemical Group	Boiling point at ambient pressure (K)		Consensus
		Review	Recommended	
m-Xylene	BTEX	412.2 [b], 412.3 [c, g, h], 412.5 [a, d, e]	412.5	High
o-Xylene	BTEX	417.0 [g], 417.2 [d], 417.6 [a, e, h], 417.7 [b, c]	417.6	High
p-Xylene	BTEX	410.7 [d], 411.4 [b, g], 411.5 [c, \e, h]	411.5	High

Notes

[a] HOWARD, P.H., 1990. [b] LIDE, D.R., 2008. [c] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [d] MERCK, 2006. [e] MONTGOMERY, J.H., 2007. [f] MONTGOMERY, J.H., 1997. [g] NIST, 2005. [h] OECD, 2000.

sub – chemical sublimes from solid to gas

dec – chemical decomposes below boiling point

low P – boiling points reported are at low air pressures

Table A2: Critical point temperature (K)

Chemical	Chemical Group	Critical point temperature (K)		Consensus
		Review	Recommended	
Aldrin	Pesticide		none	
Atrazine	Pesticide		none	
Azinphos-methyl	Pesticide		none	
Benzene	BTEX	562.0 [c], 562.1 [a]	562.0	Low
Benzo[*a*]anthracene	PAH		none	
Benzo[*b*]fluoranthene	PAH		none	
Benzo[*k*]fluoranthene	PAH		none	
Benzo[*ghi*]perylene	PAH		none	
Benzo[*a*]pyrene	PAH		none	
Carbon disulphide		552.0 [a, c], 553.2 [b]	552.0	Low
Chlorobenzene	Chlorobenzene	632.4 [c], 633.4 [a]	633.4	Low
Chloroethene		429.2 [d], 432.0 [a]	432.0	Low
2-Chlorophenol	Chlorophenol		none	
α-Chlorotoluene	Chlorotoluene		none	
2-Chlorotoluene	Chlorotoluene		none	
Chrysene	PAH		none	
p,p'-DDT	Pesticide		none	
o,p'-DDT	Pesticide		none	
Dibenz[*ah*]anthracene	PAH		none	
1,2-Dichlorobenzene	Chlorobenzene		none	

Chemical	Chemical Group	Critical point temperature (K)		Consensus
		Review	Recommended	
1,3-Dichlorobenzene	Chlorobenzene	685.7 [a]	685.7	Very Low
1,4-Dichlorobenzene	Chlorobenzene		none	
1,2-Dichloroethane		561.0 [a], 562.0 [c]	561.0	Low
2,4-Dichlorophenol	Chlorophenol		none	
Dichlorvos	Pesticide		none	
Dieldrin	Pesticide		none	
Endosulfan (α form)	Pesticide		none	
Endosulfan (β form)	Pesticide		none	
Ethylbenzene	BTEX	617.0 [c], 617.2 [a]	617.2	Low
Fenitrothion	Pesticide		none	
Fluoranthene	PAH		none	
Hexachlorobenzene	Chlorobenzene		none	
Hexchloro-1,3-butadiene			none	
α-Hexachlorocyclohexane	Pesticide		none	
β-Hexachlorocyclohexane	Pesticide		none	
γ-Hexachlorocyclohexane	Pesticide		none	
Indeno[*123-cd*]pyrene	PAH		none	
Malathion	Pesticide		none	
Naphthalene	PAH	748.0 [c], 748.4 [a]	748.4	Low
Pentachlorobenzene	Chlorobenzene		none	
Pentachlorophenol	Chlorophenol		none	
Phenol		694.2 [a], 694.3 [c]	694.2	Low
2-Propanone		508.0 [c], 508.1 [a]	508.1	Low
Pyrene	PAH		none	
1,2,3,4-Tetrachlorobenzene	Chlorobenzene		none	
1,2,3,5-Tetrachlorobenzene	Chlorobenzene		none	
1,2,4,5-Tetrachlorobenzene	Chlorobenzene		none	
1,1,1,2-Tetrachloroethane			none	
1,1,2,2-Tetrachloroethane		644.5 [c], 661.2 [a]	661.2	Low
Tetrachloroethene		620.0 [c],620.2 [a]	620.2	Low
Tetrachloromethane		556.4 [c], 556.6 [a]	556.6	Low
2,3,4,6-Tetrachlorophenol	Chlorophenol		none	
Tetraethyl lead			none	
Toluene	BTEX	591.8 [a], 593.0 [c]	591.8	Low
Tributyl tin oxide (TBTO)			none	

Chemical	Chemical Group	Critical point temperature (K)		Consensus
		Review	Recommended	
1,2,3-Trichlorobenzene	Chlorobenzene		none	
1,2,4-Trichlorobenzene	Chlorobenzene	730.7 [d]	730.7	Very Low
1,3,5-Trichlorobenzene	Chlorobenzene		none	
1,1,1-Trichloroethane		545.0 [a], 548.4 [c]	545.0	Low
Trichloroethene		544.2 [a], 571.0 [c]	544.2	Low
Trichloromethane		536.4 [a], 537.0 [c]	536.4	Low
2,4,6-Trichlorophenol	Chlorophenol		none	
α,α,α-Trichlorotoluene	Chlorotoluene		none	
Trifluralin	Pesticide		none	
m-Xylene	BTEX	617.0 [a], 618.0 [c]	617.0	Low
o-Xylene	BTEX	630.3 [a], 631.0 [c]	630.3	Low
p-Xylene	BTEX	616.2 [a], 617.0 [c]	616.2	Low

Notes

[a] LIDE, D.R., 2008. [b] MERCK, 2006. [c] NIST, 2005. [d] OECD, 2000.

Table A3: Enthalpy of vaporisation at normal boiling point (kJ mol^{-1})

Chemical	Chemical Group	Enthalpy of vaporisation at normal boiling point (kJ mol^{-1})		Consensus
		Review	Recommended	
Aldrin	Pesticide		none	
Atrazine	Pesticide		none	
Azinphos-methyl	Pesticide	96.65 [b]	96.65	Very Low
Benzene	BTEX	30.72 [a, c], 30.73 [b]	30.72	Low
Benzo[*a*]anthracene	PAH		none	
Benzo[*b*]fluoranthene	PAH		none	
Benzo[*k*]fluoranthene	PAH		none	
Benzo[*ghi*]perylene	PAH		none	
Benzo[*a*]pyrene	PAH		none	
Carbon disulphide		26.74 [a, b, c]	26.74	Low
Chlorobenzene	Chlorobenzene	35.19 [a, c]	35.19	Low
Chloroethene		20.80 [a, b]	20.80	Low
2-Chlorophenol	Chlorophenol	40.05 [b]	40.05	Very Low
α-Chlorotoluene	Chlorotoluene		none	

Chemical	Chemical Group	Enthalpy of vaporisation at normal boiling point (kJ mol^{-1})		Consensus
		Review	Recommended	
2-Chlorotoluene	Chlorotoluene	37.50 [a]	37.50	Very Low
Chrysene	PAH		none	
p,*p*'-DDT	Pesticide		none	
o,*p*'-DDT	Pesticide		none	
Dibenz[*ah*]anthracene	PAH		none	
1,2-Dichlorobenzene	Chlorobenzene	39.66 [a]	39.66	Very Low
1,3-Dichlorobenzene	Chlorobenzene	38.62 [a]	38.62	Very Low
1,4-Dichlorobenzene	Chlorobenzene	38.79 [a]	38.79	Very Low
1,2-Dichloroethane		31.98 [a, c], 32.02 [b]	31.98	Low
2,4-Dichlorophenol	Chlorophenol	36.78 [c]	36.78	Very Low
Dichlorvos	Pesticide		none	
Dieldrin	Pesticide	76.60 [b]	76.60	Very Low
Endosulfan (α form)	Pesticide		none	
Endosulfan (β form)	Pesticide		none	
Ethylbenzene	BTEX	35.20 [b], 35.57 [a, c]	35.57	Low
Fenitrothion	Pesticide		none	
Fluoranthene	PAH		none	
Hexachlorobenzene	Chlorobenzene		none	
Hexchloro-1,3-butadiene			none	
α-Hexachlorocyclohexane	Pesticide		none	
β-Hexachlorocyclohexane	Pesticide		none	
γ-Hexachlorocyclohexane	Pesticide		none	
Indeno[*123-cd*]pyrene	PAH		none	
Malathion	Pesticide		none	
Naphthalene	PAH	43.20 [a]	43.20	Very Low
Pentachlorobenzene	Chlorobenzene		none	
Pentachlorophenol	Chlorophenol		none	
Phenol		45.69 [a], 46.27 [b]	45.69	Low
2-Propanone		29.10 [a, c]	29.10	Low
Pyrene	PAH		none	
1,2,3,4-Tetrachlorobenzene	Chlorobenzene		none	
1,2,3,5-Tetrachlorobenzene	Chlorobenzene		none	
1,2,4,5-Tetrachlorobenzene	Chlorobenzene		none	
1,1,1,2-Tetrachloroethane		34.78 [b]	34.78	Very Low
1,1,2,2-Tetrachloroethane		37.64 [a, c], 38.65 [b]	37.64	Low

Chemical	Chemical Group	Enthalpy of vaporisation at normal boiling point (kJ mol^{-1})		Consensus
		Review	Recommended	
Tetrachloroethene		34.68 [a, c], 34.72 [b]	34.68	Low
Tetrachloromethane		29.82 [a, c], 29.96 [b]	29.82	Low
2,3,4,6-Tetrachlorophenol	Chlorophenol		none	
Tetraethyl lead		56.60 [c]	56.60	Very Low
Toluene	BTEX	33.18 [a, b, c]	33.18	Low
Tributyl tin oxide (TBTO)			none	
1,2,3-Trichlorobenzene	Chlorobenzene		none	
1,2,4-Trichlorobenzene	Chlorobenzene		none	
1,3,5-Trichlorobenzene	Chlorobenzene		none	
1,1,1-Trichloroethane		29.71 [b], 29.86 [a, c]	29.86	Low
Trichloroethene		31.40 [a, c], 31.47 [b]	31.40	Low
Trichloromethane		29.24 [a, c], 29.37 [b]	29.24	Low
2,4,6-Trichlorophenol	Chlorophenol		none	
α,α,α-Trichlorotoluene	Chlorotoluene		none	
Trifluralin	Pesticide		none	
m-Xylene	BTEX	35.66 [a, c], 36.36 [b]	35.66	Low
o-Xylene	BTEX	36.24 [a, c], 36.82 [b]	36.24	Low
p-Xylene	BTEX	35.67 [a, c], 35.98 [b]	35.67	Low

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] NIST, 2005.

Table A4: Henry's law constant at specific temperature (Pa m^3 mol^{-1})

Chemical	Chemical Group	Henry's law constant at 25 °C unless stated (Pa m^3 mol^{-1})		Consensus
		Review	Recommended	
Aldrin	Pesticide	2.8 [f], 22.4 [d], 50.3 [c, e], 91.2 [b]	50.3	Low
Atrazine	Pesticide	2.66E-04 (20) [c], 2.88E-04 [b], 3.08E-04 (20) [e]	2.88E-04	Very Low
Azinphos-methyl	Pesticide	1.52E-05 (20) [c], 3.17E-04 [b], 7.60E-04 (20) [e]	3.17E-04	Very Low
Benzene	BTEX	432 (NA) [g], 550 (NA) [c], 525 [d], 557 [a, b, f]	557	Medium
Benzo[*a*]anthracene	PAH	0.580 [a], 0.581 [b], 1.22 [d]	0.580	Low
Benzo[*b*]fluoranthene	PAH	0.048 (20) [b], 0.051 [d]	0.051	Low
Benzo[*k*]fluoranthene	PAH	0.016 [b], 0.043 [d]	0.043	Very Low

Chemical	Chemical Group	Henry's law constant at 25 °C unless stated (Pa m^3 mol^{-1})		Consensus
		Review	Recommended	
Benzo[*ghi*]perylene	PAH	0.027 [d], 0.033 [f], 0.048 (20) [b], 0.075 [a]	0.075	Very Low
Benzo[*a*]pyrene	PAH	0.046 [b, f], 0.047 [a], 0.050 [d]	0.046	Low
Carbon disulphide		142 (20) [c], 1350 (20 – 22) [e], 1750 [b], 1820 [f], 2.46E+06 (24) [d]	1750	Low
Chlorobenzene	Chlorobenzene	320 [a], 350 (NA) [c] 363 [d], 367 [b], 371 [f]	367	Low
Chloroethene		1080 (NA) [c], 2680 [a], 2690 [d], 2710 [f], 2817 (24.8) [g], 8020 [b]	2690	Low
2-Chlorophenol	Chlorophenol	0.057 (NA) [c], 0.653 (20) [d], 0.688 [b], 0.836 [f]	0.653 (20)	Low
α-Chlorotoluene	Chlorotoluene	34.5 (20 – 22) [c], 36.0 (20) [b], 36.2 (20) [d], 62.7 [f]	36.0 (20)	Low
2-Chlorotoluene	Chlorotoluene	137 [f], 295 (20) [b], 368 [d], 470.5 (NA) [g]	295 (20)	Very Low
Chrysene	PAH	0.065 [a, b], 0.530 [d]	0.065	Low
p,*p*'-DDT	Pesticide	0.903 [d], 1.31 (23) [e], 2.36 [b], 5.28 [f]	0.903	Very Low
o,*p*'-DDT	Pesticide	0.347 [b]	0.347	Very Low
Dibenz[*ah*]anthracene	PAH	1.72E-04 [b], 0.172 [d]	0.172	Very Low
1,2-Dichlorobenzene	Chlorobenzene	122 (20) [c], 176 [d], 178 [b], 193 [g], 195 [a], 205 [f]	195	Low
1,3-Dichlorobenzene	Chlorobenzene	182 (20) [c], 284 [d], 318 [b], 334 [f], 376 [a]	318	Low
1,4-Dichlorobenzene	Chlorobenzene	152 (20) [c], 242 [b], 244 [a], 253 [d], 295 [f]	244	Low
1,2-Dichloroethane		99 (NA) [c], 119 [d], 120 [g], 121 [b], 124 [f], 140 [a]	121	Low
2,4-Dichlorophenol	Chlorophenol	0.327 [d], 0.435 [b], 0.6 (20) [g]	0.327	Very Low
Dichlorvos	Pesticide	5.59E-03 [d], 0.097 [c], 0.194 [b], 507 (NA) [e]	5.59E-03	Very Low
Dieldrin	Pesticide	1.09 [f], 1.12 [b], 1.80 [d], 5.88 [c, e]	5.88	Low
Endosulfan (α form)	Pesticide	1.06 [b], 1.13 (NA) [c], 7.68 [d], 10.2 [e]	7.68	Very Low
Endosulfan (β form)	Pesticide	1.06 [b], 1.13 (NA) [c], 1.94 [e], 5.12 [d]	5.12	Very Low
Ethylbenzene	BTEX	731 [d], 772 [f], 798 (NA) [g], 843 [a], 855 (NA) [c], 887 [b]	843	Low
Fenitrothion	Pesticide	1.20E-03 [b], 0.037 [f], 0.095 (20) [d]	0.095 (20)	Very Low
Fluoranthene	PAH	0.912 [f], 0.957 [b], 0.960 [a], 1.47 [d]	0.960	Low
Hexachlorobenzene	Chlorobenzene	84.0 [d], 131 [a, b], 132 (23) [c], 205 [f], 719 (20) [e]	131	Low
Hexchloro-1,3-butadiene		1030 [f], 1040 (NA) [c], 1280 [d], 1630 [b]	1030	Low
α-Hexachlorocyclohexane	Pesticide	0.060 [d], 0.537 (20) [e], 0.772 [f], 0.872 [b], 1.07 [c]	0.872	Very Low
β-Hexachlorocyclohexane	Pesticide	0.023 (20 – 25) [e], 0.045 [d], 0.116 [b]	0.045	Very Low
γ-Hexachlorocyclohexane	Pesticide	0.149 [b], 0.202 (23) [e], 0.296 [c], 0.335 [f], 0.375 [d]	0.375	Very Low

Chemical	Chemical Group	Henry's law constant at 25 °C unless stated (Pa m^3 mol^{-1})		Consensus
		Review	Recommended	
Indeno[*123-cd*]pyrene	PAH	0.029 (20) [d], 0.060 (20) [b]	0.029 (20)	Very Low
Malathion	Pesticide	4.95E-04 [d, e], 2.03E-03 (20) [c], 2.28E-03 [b], 3.71E-02 [f]	4.95E-04	Low
Naphthalene	PAH	43.0 [a, b], 53.1 [f], 53.9 [d]	43.0	Low
Pentachlorobenzene	Chlorobenzene	52.1 [d], 85.0 [a, b], 271 [f], 719 (20) [e]	85.0	Low
Pentachlorophenol	Chlorophenol	0.0279 (NA) [e], 0.079 [b], 0.151 [f], 0.279 (NA) [c]	0.079	Very Low
Phenol		0.031 [g], 0.040 (NA) [c], 0.050 [b], 0.065 [d], 0.078 [f]	0.065	Very Low
2-Propanone		3.72 (NA) [c], 3.76 [d], 3.97 [b], 4.83 [f]	3.76	Low
Pyrene	PAH	0.919 [b], 0.920 [a], 1.14 [f], 1.20 [d]	0.920	Low
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	111 [b], 141 [f], 144 [a, d]	144	Low
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	304 [f], 588 [b, d], 590 [a]	588	Low
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	101 (20) [d], 122 [a, b], 257 [f]	122	Low
1,1,1,2-Tetrachloroethane		184 (20) [d], 240 [a], 245 [c], 248 [b], 264 [f]	245	Low
1,1,2,2-Tetrachloroethane		26.0 [a], 30.8 [d], 37.2 [g], 44.6 [f], 46.1 [c], 47.0 [b]	46.1	Low
Tetrachloroethene		1510 (NA) [c], 1690 [d], 1730 [a], 1860 [f], 2670 [b]	1730	Low
Tetrachloromethane		2740 [d], 2870 [f], 2930 [b], 2990 [a], 3060 [e], 3080 [c]	2990	Medium
2,3,4,6-Tetrachlorophenol	Chlorophenol	0.355 [b]	0.355	Very Low
Tetraethyl lead			None	
Toluene	BTEX	602 (NA) [c], 607 [d], 627 [f], 660 [a], 680 [b]	660	Medium
Tributyl tin oxide (TBTO)			None	
1,2,3-Trichlorobenzene	Chlorobenzene	170 [f], 184 [d], 242 [a, b]	242	Low
1,2,4-Trichlorobenzene	Chlorobenzene	144 (NA) [c], 208.7 (NA) [g], 228 [f], 277 [a, b], 480 [d]	277	Low
1,3,5-Trichlorobenzene	Chlorobenzene	159 [f], 193 (NA) [c], 531 [d], 856 [b], 1100 [a]	1100	Very Low
1,1,1-Trichloroethane		811 (NA) [c], 1640 [f], 1710 [b], 1760 [a], 1850 [d]	1710	Low
Trichloroethene		961 [d], 1010 [f], 1030 [a], 1040 (NA) [c], 1044 (NA) [g], 1180 [b]	1030	Low
Trichloromethane		381 [b], 386 [f], 430 [a], 441 [c], 479 [d]	430	Low
2,4,6-Trichlorophenol	Chlorophenol	6.22E-03 (NA) [c], 9.19E-03 [d], 0.569 [b]	9.19E-03	Very Low
α,α,α-Trichlorotoluene	Chlorotoluene		None	
Trifluralin	Pesticide	4.90 (23) [e], 5.91 (23) [d], 10.1 [b]	5.91 (23)	Very Low
m-Xylene	BTEX	669 [f], 682 [d], 730 [a, b], 778 (NA) [c]	730	Low
o-Xylene	BTEX	467 [d], 478 [f], 517 (NA) [c], 551 [a], 565 [b]	551	Low

Chemical	Chemical Group	Henry's law constant at 25 °C unless stated (Pa m^3 mol^{-1})		Consensus
		Review	Recommended	
p-Xylene	BTEX	578 [b], 659 [d], 669 [f], 690 [a], 778 (NA) [c]	669	Low

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] HOWARD, P.H., 1990. [d] MONTGOMERY, J.H., 2007. [e] MONTGOMERY, J.H., 1997. [f] NIST, 2005. [g] OECD, 2000.

Table A5: Melting point (K)

Chemical	Chemical Group	Melting point (K)		Consensus
		Review	Recommended	
Aldrin	Pesticide	374.5 [g], 377.2 [a, b, c, d, f], 378.6 [e]	377.2	High
Atrazine	Pesticide	445.7 [c, d, f], 446.2 [a, b], 450.3 [g],	445.7	High
Azinphos-methyl	Pesticide	345.4 [g], 345.6 [f], 346.2 [a, b], 346.7 [c, d]	346.2	High
Benzene	BTEX	278.6 [a, b, g], 278.7 [c, d, e, h]	278.7	High
Benzo[*a*]anthracene	PAH	432.0 [g], 432.2 [e], 433.7 [a, b], 434.2 [d]	433.7	Medium
Benzo[*b*]fluoranthene	PAH	436.0 [e], 441.2 [a, b]	441.2	Low
Benzo[*k*]fluoranthene	PAH	485.7 [e], 490.0 [g], 490.2 [a, b]	490.2	Medium
Benzo[*ghi*]perylene	PAH	545.7 [a, b], 552.2 [e], 553.6 [g]	545.7	Medium
Benzo[*a*]pyrene	PAH	450.0 [g], 451.0 [e], 452.2 [d], 454.3 [a, b]	454.3	Medium
Carbon disulphide		161.0 [g], 161.1 [a, b], 161.6 [d], 161.7 [c, e, f]	161.7	High
Chlorobenzene	Chlorobenzene	227.6 [c, e], 227.8 [a, b], 228.0 [g], 228.2 [d]	227.8	High
Chloroethene		111.7 [g], 119.3 [a, b], 119.4 [c, d, e, h]	119.4	Medium
2-Chlorophenol	Chlorophenol	281.2 [e], 281.8 [g], 282.5 [c, d], 282.6 [a, b]	282.6	High
α-Chlorotoluene	Chlorotoluene	227.7 [c, d], 228.2 [a, b], 230.2 [h], 230.9 [g], 234.2 [e]	228.2	High
2-Chlorotoluene	Chlorotoluene	236.7 [h], 237.4 [a, b], 237.6 [d], 238.0 [g]	237.4	Medium
Chrysene	PAH	527.2 [d], 528.7 [a, b], 528.8 [e], 529.0 [g]	528.7	Medium
p,*p*'-DDT	Pesticide	381.7 [b, f], 381.9 [d], 382.8 [g], 383.0 [e]	381.7	Medium
o,*p*'-DDT	Pesticide	381.7 [b], 381.9 [d]	381.7	Low
Dibenz[*ah*]anthracene	PAH	536.7 [e], 538.6 [g], 539.2 [d], 542.7 [a, b]	542.7	Medium
1,2-Dichlorobenzene	Chlorobenzene	256.0 [g], 256.1 [d], 256.2 [a, b, c], 256.5 [h], 257.2 [e]	256.2	High
1,3-Dichlorobenzene	Chlorobenzene	248.3 [g], 248.4 [a, b, d], 248.5 [c, e]	248.4	High
1,4-Dichlorobenzene	Chlorobenzene	326.1 [e, g], 326.2 [a, b], 326.3 [c], 326.7 [h], 326.9 [d]	326.2	High
1,2-Dichloroethane		230.0 [g], 237.4 [h], 237.5 [a, b], 237.8 [c], 238.0 [e]	237.5	Medium
2,4-Dichlorophenol	Chlorophenol	316.7 [h], 317.2 [e], 318.2 [a, b, d], 319.7 [g]	318.2	Medium

Chemical	Chemical Group	Melting point (K)		Consensus
		Review	Recommended	
Dichlorvos	Pesticide		none	
Dieldrin	Pesticide	432.7 [e], 448.7 [a, b, c, f], 449.7 [d], 451.0 [g]	448.7	High
Endosulfan (α form)	Pesticide	379.2 [a, b, c, f], 381.3 [g], 382.2 [d, e]	379.2	High
Endosulfan (β form)	Pesticide	379.2 [a, c], 481.2 [b, e, f], 482.2 [d]	481.2	Medium
Ethylbenzene	BTEX	178.1 [d], 178.2 [a, b, c, h], 178.8 [e], 179.0 [g]	178.2	High
Fenitrothion	Pesticide	276.6 [b]	276.6	Very Low
Fluoranthene	PAH	382.7 [e], 383.3 [a, b], 384.2 [g]	383.3	Medium
Hexachlorobenzene	Chlorobenzene	501.7 [f], 502.0 [a, b, g], 504.2 [c, d], 505.0 [e]	502.0	High
Hexchloro-1,3-butadiene		252.2 [a, b, c, d, e]	252.2	High
α-Hexachlorocyclohexane	Pesticide	430.2 [g], 430.5 [e], 431.2 [a, b], 432.3 [f], 432.7 [c]	431.2	High
β-Hexachlorocyclohexane	Pesticide	570.0 [g], 582.2 [b], 584.9 [f], 586.3 [e]	586.3	Medium
γ-Hexachlorocyclohexane	Pesticide	385.7 [a, b, c, d, f], 387.5 [e], 398.1 [g]	385.7	High
Indeno[*123-cd*]pyrene	PAH	434.7 [e], 435.2 [a, b], 436.4 [g]	435.2	Medium
Malathion	Pesticide	274.6 [a, b], 275.4 [g], 276.0 [f], 276.1 [c, d, e]	276.1	High
Naphthalene	PAH	353.2 [g, h], 353.4 [a, b, c, d], 353.6 [e]	353.4	High
Pentachlorobenzene	Chlorobenzene	357.7 [g], 358.5 [e], 359.2 [a, b, f]	359.2	Medium
Pentachlorophenol	Chlorophenol	447.2 [a, b, f], 463.0 [g], 463.2 [c], 463.7 [d], 464.2 [e]	447.2	High
Phenol		313.7 [e], 314.0 [a, b, d, g], 314.1 [h], 316.2 [c]	314.0	High
2-Propanone		177.8 [c, e], 178.5 [a, b], 178.6 [h], 178.7 [g], 179.2 [d]	178.5	High
Pyrene	PAH	423.8 [a, b], 424.0 [g], 425.7 [e], 429.2 [d]	423.8	Medium
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	320.0 [g], 320.3 [e], 320.7 [a, b]	320.7	Medium
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	323.9 [g], 327.7 [a, b, e]	327.7	Medium
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	365.1 [g], 412.7 [a, b, e]	412.7	Low
1,1,1,2-Tetrachloroethane		203.0 [a, b, c]	203.0	Low
1,1,2,2-Tetrachloroethane		229.2 [d], 229.7 [g], 230.8 [a, b], 233.3 [h], 237.2 [c, e]	230.8	High
Tetrachloroethene		250.8 [g], 250.9 [a, b], 251.2 [d], 252.5 [e], 254.2 [c]	250.9	High
Tetrachloromethane		250.2 [c, d, e, f], 250.3 [g], 250.5 [a, b]	250.2	High
2,3,4,6-Tetrachlorophenol	Chlorophenol	341.0 [g], 343.2 [a, b]	343.2	Low
Tetraethyl lead		142.9 [g]	142.9	Very Low
Toluene	BTEX	178.1 [g], 178.2 [a, b, c, d, e, h]	178.2	High
Tributyl tin oxide (TBTO)		228.2 [a]	228.2	Very Low
1,2,3-Trichlorobenzene	Chlorobenzene	324.5 [a, b], 325.5 [g], 325.8 [d], 326.85 [e]	324.5	Medium
1,2,4-Trichlorobenzene	Chlorobenzene	287.3 [g], 289.9 [h], 290.1 [a, b], 290.2 [c, d, e]	290.2	High

Chemical	Chemical Group	Melting point (K)		Consensus
		Review	Recommended	
1,3,5-Trichlorobenzene	Chlorobenzene	335.9 [g], 336.0 [a, b], 336.6 [d], 336.7 [c, e]	336.0	High
1,1,1-Trichloroethane		240.0 [g], 240.7 [d], 242.6 [e], 242.8 [c], 243.1 [a, b]	243.1	High
Trichloroethene		188.4 [d, g], 188.5 [a, b], 186.1 [e], 191.9 [h], 200.2 [c]	188.5	High
Trichloromethane		209.7 [a, b, c, d, e], 210.0 [g]	209.7	High
2,4,6-Trichlorophenol	Chlorophenol	342.2 [a, b, c, d], 342.7 [e]	342.2	Medium
α,α,α-Trichlorotoluene	Chlorotoluene	246.1 [g], 268.2 [d], 268.4 [h], 268.7 [a, b]	268.7	Medium
Trifluralin	Pesticide	319.7 [d, f], 322.2 [a, b], 322.5 [g], 322.9 [e]	322.2	High
m-Xylene	BTEX	225.0 [g], 225.3 [h], 225.4 [a, b], 225.5 [e], 225.8 [c, d]	225.4	High
o-Xylene	BTEX	248.0 [a, b, e, g, h], 248.2 [c, d]	248.0	High
p-Xylene	BTEX	286.4 [a, b, g], 286.5 [h], 286.7 [c, d, e]	286.4	High

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] HOWARD, P.H., 1990. [d] MERCK, 2006. [e] MONTGOMERY, J.H., 2007. [f] MONTGOMERY, J.H., 1997. [g] NIST, 2005. [h] OECD, 2000.

Table A6: Molecular weight (g mol^{-1})

Chemical	Chemical Group	Relative molecular weight (g mol^{-1})		Consensus
		Review	Recommended	
Aldrin	Pesticide	364.91 [a, b, c, d, g], 364.92 [e, f], 364.93 [c]	364.91	High
Atrazine	Pesticide	84.08 [e], 215.68 [a, b, c, d, f, g]	215.68	High
Azinphos-methyl	Pesticide	317.32 [a, b, d], 317.33 [e, f, g], 317.34 [c]	317.32	High
Benzene	BTEX	78.11 [a, b, c, d, e, g]	78.11	Very High
Benzo[*a*]anthracene	PAH	228.29 [a, b, d, g], 228.30 [e]	228.29	Medium
Benzo[*b*]fluoranthene	PAH	252.31 [a, b, g], 252.32 [e]	252.31	Medium
Benzo[*k*]fluoranthene	PAH	252.31 [a, b, g], 252.32 [e]	252.31	Medium
Benzo[*ghi*]perylene	PAH	276.33 [a, b, g], 276.34 [e]	276.33	Medium
Benzo[*a*]pyrene	PAH	252.31 [a, b, d, g], 252.32 [e]	252.31	Medium
Carbon disulphide		76.13 [c, e, f], 76.14 [a, b, d, g]	76.14	High
Chlorobenzene	Chlorobenzene	112.56 [a, b, c, d, e, g]	112.56	Very High
Chloroethene		62.50 [a, b, c, d, e, g]	62.50	Very High
2-Chlorophenol	Chlorophenol	128.56 [a, b, c, d, e, g]	128.56	Very High
α-Chlorotoluene	Chlorotoluene	126.58 [a, b, c, d, g], 126.59 [e, h]	126.58	High
2-Chlorotoluene	Chlorotoluene	126.58 [a, b, d, g]	126.58	Medium
Chrysene	PAH	228.29 [a, b, d, g], 228.30 [e]	228.29	Medium

Chemical	Chemical Group	Relative molecular weight (g mol^{-1})		Consensus
		Review	Recommended	
p,p'-DDT	Pesticide	354.48 [g], 354.49 [b, d, e, f]	354.49	Medium
o,p'-DDT	Pesticide	354.48 [g], 354.49 [b, d]	354.49	Low
Dibenz[*ah*]anthracene	PAH	278.35 [a, b, d, g], 278.36 [e]	278.35	Medium
1,2-Dichlorobenzene	Chlorobenzene	147.00 [a, b, d, e, g], 147.01 [c]	147.00	High
1,3-Dichlorobenzene	Chlorobenzene	147.00 [a, b, d, e, g], 147.01 [c]	147.00	High
1,4-Dichlorobenzene	Chlorobenzene	147.00 [a, b, d, e, g], 147.01 [c]	147.00	High
1,2-Dichloroethane		98.96 [a, b, c, e, g, h]	98.96	Very High
2,4-Dichlorophenol	Chlorophenol	163.00 [a, b, d, e, g, h]	163.00	Very High
Dichlorvos	Pesticide	220.98 [a, b, c, d, e, f, g]	220.98	Very High
Dieldrin	Pesticide	380.91 [a, b, d, e, f, g], 380.93 [c]	380.91	High
Endosulfan (α form)	Pesticide	406.92 [e, f, g], 406.93 [a, b, d], 406.95 [c]	406.93	High
Endosulfan (β form)	Pesticide	406.92 [e, f, g], 406.93 [a, b, d], 406.95 [c]	406.93	High
Ethylbenzene	BTEX	106.16 [c], 106.17 [a, b, d, e, g], 106.2 [h]	106.17	High
Fenitrothion	Pesticide	277.23 [a, b, d], 277.24 [g]	277.23	Medium
Fluoranthene	PAH	202.25 [a, b, g], 202.26 [e]	202.25	Medium
Hexachlorobenzene	Chlorobenzene	284.78 [a, b, d, e, f, g], 284.80 [c]	284.78	High
Hexchloro-1,3-butadiene		260.76 [a, b, c, d, e, g]	260.76	Very High
α-Hexachlorocyclohexane	Pesticide	290.83 [a, b, e, f, g], 290.85 [c]	290.83	High
β-Hexachlorocyclohexane	Pesticide	290.83 [a, b, e, f, g]	290.83	High
γ-Hexachlorocyclohexane	Pesticide	290.83 [a, b, d, e, f, g], 290.85 [c]	290.83	High
Indeno[*123-cd*]pyrene	PAH	276.33 [a, b, g], 276.34 [e]	276.33	Medium
Malathion	Pesticide	330.36 [a, b, c, d, e, f, g]	330.36	Very High
Naphthalene	PAH	128.16 [c], 128.17 [a, b, d, g], 128.18 [e]	128.17	High
Pentachlorobenzene	Chlorobenzene	250.34 [a, b, e, f, g]	250.34	High
Pentachlorophenol	Chlorophenol	266.34 [a, b, d, e, f, g], 266.35 [c]	266.34	High
Phenol		94.11 [a, b, c, d, e, g]	94.11	Very High
2-Propanone		58.08 [a, b, d, e, g, h], 58.09 [c]	58.08	Very High
Pyrene	PAH	202.25 [a, b, d, g], 202.26 [e]	202.25	Medium
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	215.89 [a, b, e, g]	215.89	Medium
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	215.89 [a, b, e, g]	215.89	Medium
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	215.89 [a, b, e, g]	215.89	Medium
1,1,1,2-Tetrachloroethane		167.85 [a, b, c, e, g]	167.85	High
1,1,2,2-Tetrachloroethane		167.85 [a, b, d, e, g, h], 167.86 [c]	167.85	Very High
Tetrachloroethene		165.82 [c], 165.83 [a, b, d, e, g]	165.83	High
Tetrachloromethane		153.82 [a, b, d, e, f, g], 153.84 [c]	153.82	High

Chemical	Chemical Group	Relative molecular weight ($g\ mol^{-1}$)		Consensus
		Review	Recommended	
2,3,4,6-Tetrachlorophenol	Chlorophenol	231.89 [a, b, g]	231.89	Low
Tetraethyl lead		323.40 [a], 323.44 [d, g]	323.44	Low
Toluene	BTEX	92.13 [c], 92.14 [a, b, d, e, g]	92.14	High
Tributyl tin oxide (TBTO)		596.11 [a, g]	596.11	Low
1,2,3-Trichlorobenzene	Chlorobenzene	181.45 [a, b, d, e, g]	181.45	High
1,2,4-Trichlorobenzene	Chlorobenzene	181.45 [a, b, d, e, g], 181.46 [c]	181.45	High
1,3,5-Trichlorobenzene	Chlorobenzene	181.45 [a, b, c, d, e, g]	181.45	Very High
1,1,1-Trichloroethane		133.40 [a, b, d, e, g], 133.42 [c]	133.40	High
Trichloroethene		131.39 [a, b, d, e, g], 131.40 [c]	131.39	High
Trichloromethane		119.38 [a, b, d, e, g], 119.39 [c]	119.38	High
2,4,6-Trichlorophenol	Chlorophenol	197.45 [a, b, c, d, e, g]	197.45	Very High
α,α,α-Trichlorotoluene	Chlorotoluene	195.47 [a, b, d, g], 195.48 [c, h]	195.47	High
Trifluralin	Pesticide	335.28 [a, b, d, g], 335.29 [e, f]	335.28	High
m-Xylene	BTEX	106.17 [a, b, c, d, e, g]	106.17	Very High
o-Xylene	BTEX	106.16 [c], 106.17 [a, b, d, e, g]	106.17	High
p-Xylene	BTEX	106.17 [a, b, c, d, e, g]	106.17	Very High

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] HOWARD, P.H., 1990. [d] MERCK, 2006. [e] MONTGOMERY, J.H., 2007. [f] MONTGOMERY, J.H., 1997. [g] NIST, 2005. [h] OECD, 2000.

Table A7: Octanol-water partition coefficient (dimensionless)

Chemical	Chemical Group	Octanol-water partition coefficient (log value, dimensionless)		Consensus
		Review	Recommended	
Aldrin	Pesticide	3.01 [b], 6.47 [d], 6.50 [c], 5.17 – 7.40 [e]	6.47	Low
Atrazine	Pesticide	2.27 [e], 2.42 [d], 2.75 [b, c]	2.75	Low
Azinphos-methyl	Pesticide	2.69 [d], 2.70 [b], 2.72 [e], 2.75 [c]	2.69	Low
Benzene	BTEX	2.10 [d], 2.13 [a, b, c, f]	2.13	Medium
Benzo[*a*]anthracene	PAH	5.50 [d], 5.91 [a, b]	5.91	Low
Benzo[*b*]fluoranthene	PAH	5.80 [b], 6.08 [d]	6.08	Low
Benzo[*k*]fluoranthene	PAH	6.00 [b], 6.26 [d]	6.26	Low
Benzo[*ghi*]perylene	PAH	6.50 [b], 6.81 [d], 6.90 [a]	6.81	Low
Benzo[*a*]pyrene	PAH	6.04 [b], 6.18 [d], 6.20 [a]	6.18	Low
Carbon disulphide		1.70 – 4.16 [c], 1.94 [d], 2.00 [e], 2.04 [b]	2.00	Low
Chlorobenzene	Chlorobenzene	2.80 [b], 2.84 [a, c], 2.87 [d]	2.84	Medium

Chemical	Chemical Group	Octanol-water partition coefficient (log value, dimensionless)		Consensus
		Review	**Recommended**	
Chloroethene		0.60^{d}, $1.38^{a, b, c}$, 1.58^{f}	1.38	Low
2-Chlorophenol	Chlorophenol	2.12^{d}, 2.15^{c}, 2.17^{b}	2.15	Low
α-Chlorotoluene	Chlorotoluene	$2.30^{c, d}$, 2.66^{f}	2.30	Low
2-Chlorotoluene	Chlorotoluene	$3.42^{a, d, f}$, 3.49^{b}	3.42	Low
Chrysene	PAH	5.60^{b}, 5.73^{a}, 5.83^{d}	5.73	Low
p,*p*'-DDT	Pesticide	$4.89 – 6.91^{e}$, 6.11^{d}, 6.19^{b}	6.11	Low
o,*p*'-DDT	Pesticide		none	
Dibenz[*ah*]anthracene	PAH	6.38^{d}, 6.75^{b}	6.38	Low
1,2-Dichlorobenzene	Chlorobenzene	$3.38^{a, c}$, $3.40^{b, f}$, 3.47^{d}	3.38	Medium
1,3-Dichlorobenzene	Chlorobenzene	3.40^{b}, 3.48^{a}, 3.51^{d}, 3.60^{c}	3.48	Medium
1,4-Dichlorobenzene	Chlorobenzene	3.38^{a}, $3.40^{b, d}$, 3.52^{c}	3.40	Medium
1,2-Dichloroethane		1.45^{f}, $1.48^{a, b, c, d}$	1.48	Medium
2,4-Dichlorophenol	Chlorophenol	3.14^{d}, 3.20^{b}, $3.23^{a, f}$	3.23	Medium
Dichlorvos	Pesticide	1.16^{c}, 1.34^{d}, $1.40 – 2.29^{d}$, 1.45^{b}	1.34	Very Low
Dieldrin	Pesticide	$3.69 – 6.20^{e}$, 4.32^{c}, 4.94^{d}, 5.20^{b},	4.94	Very Low
Endosulfan (α form)	Pesticide	3.55^{e}, 3.62^{b}, 3.69^{d}, 3.83^{c}	3.69	Medium
Endosulfan (β form)	Pesticide	$3.62^{d, e}$, 3.83^{b}	3.62	Low
Ethylbenzene	BTEX	3.13^{b}, $3.15^{a, c, f}$, 3.21^{d}	3.15	Medium
Fenitrothion	Pesticide	3.40^{b}, 3.44^{d}	3.44	Low
Fluoranthene	PAH	5.07^{a}, 5.13^{d}, 5.22^{b}	5.13	Low
Hexachlorobenzene	Chlorobenzene	$3.93 – 6.42^{e}$, 5.31^{c}, 5.47^{a}, 5.50^{b}, 5.68^{d}	5.47	Medium
Hexchloro-1,3-butadiene		4.70^{b}, 4.86^{d}, 4.90^{c}	4.86	Low
α-Hexachlorocyclohexane	Pesticide	3.68^{e}, 3.77^{d}, 3.80^{c}, 3.81^{b}	3.77	Medium
β-Hexachlorocyclohexane	Pesticide	3.80^{b}, 3.87^{d}, 4.15^{e}	3.87	Low
γ-Hexachlorocyclohexane	Pesticide	3.55^{e}, 3.61^{c}, 3.67^{d}, 3.70^{b}	3.67	Medium
Indeno[*123-cd*]pyrene	PAH	5.97^{d}, 7.53^{b}	5.97	Very Low
Malathion	Pesticide	2.36^{c}, 2.63^{e}, 2.80^{b}, 2.90^{d}	2.90	Low
Naphthalene	PAH	3.30^{c}, 3.34^{a}, 3.35^{d}, 3.37^{b}, 3.39^{f}	3.34	Medium
Pentachlorobenzene	Chlorobenzene	5.00^{b}, 5.03^{a}, 5.11^{d}, 5.32^{e}	5.03	Medium
Pentachlorophenol	Chlorophenol	$3.32 – 5.86^{e}$, 4.71^{d}, 5.05^{b}, 5.07^{a}, 5.12^{c}	5.07	Low
Phenol		$1.46^{b, c}$, 1.47^{f}, $1.48^{a, d}$	1.48	Medium
2-Propanone		$-0.24^{a, b, c, d, f}$	-0.24	High
Pyrene	PAH	5.03^{d}, 5.08^{a}, 5.18^{b}	5.08	Low
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	4.50^{b}, 4.54^{d}, 4.55^{a}	4.54	Low

Chemical	Chemical Group	Octanol-water partition coefficient (log value, dimensionless)		Consensus
		Review	Recommended	
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	4.50 [b], 4.58 [d], 4.65 [a]	4.58	Low
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	4.50 [b], 4.51 [a], 4.59 [d]	4.51	Low
1,1,1,2-Tetrachloroethane		3.03 [b, c]	3.03	Low
1,1,2,2-Tetrachloroethane		2.39 [a, b, c, f], 2.48 [d]	2.39	Medium
Tetrachloroethene		2.55 [d], 2.88 [a, b], 3.40 [c]	2.88	Low
Tetrachloromethane		2.64 [a], 2.67 [d], 2.78 [e], 2.83 [b, c]	2.83	Medium
2,3,4,6-Tetrachlorophenol	Chlorophenol	4.42 [d], 4.45 [b]	4.42	Low
Tetraethyl lead			none	
Toluene	BTEX	2.67 [d], 2.68 [f], 2.69 [b], 2.73 [a, c]	2.73	Medium
Tributyl tin oxide (TBTO)			none	
1,2,3-Trichlorobenzene	Chlorobenzene	4.04 [a], 4.09 [d], 4.10 [b]	4.09	Low
1,2,4-Trichlorobenzene	Chlorobenzene	3.98 [a], 4.02 [c], 4.03 [d], 4.04 [f], 4.10 [b]	4.03	Medium
1,3,5-Trichlorobenzene	Chlorobenzene	4.02 [a]. 4.10 [b], 4.15 [d], 4.49 [c]	4.10	Low
1,1,1-Trichloroethane		2.38 [d], 2.49 [a, b, c]	2.49	Medium
Trichloroethene		2.34 [f], 2.42 [c], 2.53 [a, b], 2.64 [d]	2.53	Medium
Trichloromethane		1.97 [a, b, c], 2.08 [d]	1.97	Low
2,4,6-Trichlorophenol	Chlorophenol	3.52 [d], 3.69 [b, c]	3.69	Low
α,α,α-Trichlorotoluene	Chlorotoluene	2.92 [b, c, d, f]	2.92	Medium
Trifluralin	Pesticide	5.23 [d, e], 5.34 [b]	5.23	Low
m-Xylene	BTEX	3.20 [a, b, c, f], 3.26 [d]	3.20	Medium
o-Xylene	BTEX	3.12 [a, c, d, f], 3.15 [b]	3.12	Medium
p-Xylene	BTEX	3.15 [a, c, f], 3.18 [b], 3.26 [d]	3.15	Medium

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] HOWARD, P.H., 1990. [d] MONTGOMERY, J.H., 2007. [e] MONTGOMERY, J.H., 1997. [f] OECD, 2000.

Table A8: Vapour pressure at specific temperature (Pa)

Chemical	Chemical Group	Vapour pressure at 25°C unless stated (Pa)		Consensus
		Review	Recommended	
Aldrin	Pesticide	0.005 (20) [c], 0.005 [b], 0.01 (20) [d], 0.020 [f], 0.023 [e]	0.005	Low
Atrazine	Pesticide	3.71E-05 (20) [c], 4.00E-05 (20) [f], 4.00E-05 [b]	4.00E-05	Low
Azinphos-methyl	Pesticide	1.00E-06 (20) [c], 3.00E-05 [b], 2.13E-04 (20) [f]	3.00E-05	Very Low

Chemical	Chemical Group	Vapour pressure at 25°C unless stated (Pa)		Consensus
		Review	Recommended	
Benzene	BTEX	9970 (20) [g], 10000 (20) [a], 12600 [e], 12700 [b, c]	12700	Low
Benzo[*a*]anthracene	PAH	1.45E-05 [e], 2.80E-05 [b]	2.80E-5	Very Low
Benzo[*b*]fluoranthene	PAH	1.03E-06 [b], 6.67E-05 (20) [e]	6.67E-05 (20)	Very Low
Benzo[*k*]fluoranthene	PAH	1.28E-08 [e], 5.20E-08 [b]	1.28E-08	Very Low
Benzo[*ghi*]perylene	PAH	1.43E-08 [e], 3.12E-08 [b]	1.43E-08	Very Low
Benzo[*a*]pyrene	PAH	7.00E-07 [b], 3.05E-06 [e]	3.05E-06	Very Low
Carbon disulphide		39600 (20) [c], 39700 (20) [f], 48000 [e], 48200 [b]	48000	Low
Chlorobenzene	Chlorobenzene	1580 [b, e], 1590 [c]	1580	Low
Chloroethene		333000 (20) [g], 337000 (20) [d], 355000 [b, c, e]	355000	Medium
2-Chlorophenol	Chlorophenol	132 [b], 189 [c], 239 [e]	239	Very Low
α-Chlorotoluene	Chlorotoluene	100 (17.7) [a], 133 (22) [c], 173 [e], 215 [b], 930 [g]	173	Very Low
2-Chlorotoluene	Chlorotoluene	100 (3.0) [a], 360 (20) [g], 478 [b]	478	Very Low
Chrysene	PAH	5.70E-07 [b], 6.93E-07 [e]	6.93E-07	Very Low
p,*p*'-DDT	Pesticide	1.96E-05 [e], 2.00E-05 (20) [d], 2.00E-05 [b], 5.73E-05 [f]	2.00E-05	Low
o,*p*'-DDT	Pesticide	2.00E-05 (20) [d], 2.53E-05 [b]	2.00E-05 (20)	Very Low
Dibenz[*ah*]anthracene	PAH	3.70E-10 [b], 3.71E-10 [e]	3.71E-10	Low
1,2-Dichlorobenzene	Chlorobenzene	100 (16.3) [a], 170 [b], 196 [c, g], 200 [e], 208 [d]	196	Low
1,3-Dichlorobenzene	Chlorobenzene	100 (8.0) [a], 260 [b], 281 [e], 307 [c]	281	Very Low
1,4-Dichlorobenzene	Chlorobenzene	53.3 [d], 70.7 [e], 100 (8.0) [a], 130 [b], 235 [c], 1330 (54.8) [g]	70.7	Very Low
1,2-Dichloroethane		8130 (20) [g], 10000 (23.7) [a], 10500 (20) [c], 10500 [b], 11300 [e]	10500	Low
2,4-Dichlorophenol	Chlorophenol	11.9 [e], 12.0 [b], 16.0 [g]	11.9	Low
Dichlorvos	Pesticide	1.60 (20) [d], 7.02 [b], 7.03 [c, e, f]	7.03	Medium
Dieldrin	Pesticide	2.37E-05 (20) [f], 4.13E-04 (20) [d], 5.00E-04 [b], 5.00E-04 (20) [c], 7.80E-04 [e]	5.00E-04	Low
Endosulfan (α form)	Pesticide	1.30E-03 [b], 1.33E-03 [c], 6.11E-03 [e, f]	6.11E-03	Low
Endosulfan (β form)	Pesticide	1.33E-03 [c], 3.20E-03 [e, f], 6.10E-03 [b]	3.20E-03	Low
Ethylbenzene	BTEX	1000 (21.1) [a], 1270 [b, c, g], 1280 [e]	1270	Medium
Fenitrothion	Pesticide	1.30E-04 [b], 8.00E-04 (20) [d]	8.00E-04 (20)	Very Low
Fluoranthene	PAH	1.23E-03 [b], 3.13E-03 [e]	3.13E-03	Very Low
Hexachlorobenzene	Chlorobenzene	1.45E-03 (20) [d, f], 2.30E-03 [b], 2.33E-03 [e], 2.53E-03 [c]	1.45E-03 (20)	Low

Chemical	Chemical Group	Vapour pressure at 25°C unless stated (Pa)		Consensus
		Review	Recommended	
Hexchloro-1,3-butadiene		10 (22) [a], 20 (20) [e], 20 [b, c]	20	Low
α-Hexachlorocyclohexane	Pesticide	3.00E-03 [b], 6.00E-03 [c], 0.231 [e, f]	0.231	Low
β-Hexachlorocyclohexane	Pesticide	3.73E-05 (20) [f], 4.00E-05 [b], 6.21E-05 [e]	6.21E-05	Very Low
γ-Hexachlorocyclohexane	Pesticide	1.25E-03 (20) [d, f], 3.74E-03 [b], 7.43E-03 [c], 0.011 [e]	1.25E-03 (20)	Low
Indeno[*123-cd*]pyrene	PAH	1.35E-08 [e], 3.66E-08 [b]	1.35E-08	Very Low
Malathion	Pesticide	1.67E-04 (20) [f], 1.00E-03 [b], 1.05E-03 (20) [c], 2.24E-03 [e], 5.33E-03 (30) [d]	1.00E-03	Low
Naphthalene	PAH	10.0 (24.1) [a], 10.4 [b], 10.9 [c], 11.3 [g], 14.0 [e]	10.4	Low
Pentachlorobenzene	Chlorobenzene	0.22 [b], 0.8 (20 – 30) [e, f]	0.22	Very Low
Pentachlorophenol	Chlorophenol	0.015 [c], 0.023 (20) [f], 0.035 [e], 0.038 [b]	0.035	Low
Phenol		10 (9.6) [a], 20.0 (20) [g], 47.0 [b], 55.9 [e], 69.9 [c]	55.9	Very Low
2-Propanone		10000 (1.3) [a], 30664 [g], 30800 [b, c], 31300 [e]	30800	Low
Pyrene	PAH	6.00E-04 [b], 1.65E-03 [e]	1.65E-3	Very Low
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	3.03 [e], 4.00 [b]	3.03	Very Low
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	8.64 [e], 9.80 [b]	8.64	Very Low
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	0.667 [e], 0.720 [b]	0.667	Very Low
1,1,1,2-Tetrachloroethane		1000 (17.0) [a], 1580 [b], 1600 [c]	1580	Low
1,1,2,2-Tetrachloroethane		705 [g], 793 [b], 813 [c], 867 [e]	793	Low
Tetrachloroethene		1000 (10) [a], 2420 [b], 2470 [c], 2570 [e]	2470	Low
Tetrachloromethane		10000 (15.8) [a], 12000 (20) [f], 15200 [c], 15300 [b, e]	15300	Low
2,3,4,6-Tetrachlorophenol	Chlorophenol	0.280 [b]	0.280	Very Low
Tetraethyl lead			none	
Toluene	BTEX	1000 (1.5) [a], 2950 (20) [g], 3730 [e], 3790 [c], 3800 [b]	3790	Low
Tributyl tin oxide (TBTO)			none	
1,2,3-Trichlorobenzene	Chlorobenzene	28.0 [b], 72.3 [e]	72.3	Very Low
1,2,4-Trichlorobenzene	Chlorobenzene	38.7 [c], 40.0 [b], 45.9 [g], 47.9 [e]	40.0	Low
1,3,5-Trichlorobenzene	Chlorobenzene	25.0 [b], 77.1 [c], 77.3 [e]	77.3	Low
1,1,1-Trichloroethane		10000 (14.2) [a], 16500 [b, c, e]	16500	Low
Trichloroethene		9080 [g], 10000 (26.7) [a], 9200 [c], 9770 [e], 9900 [b]	9770	Low
Trichloromethane		10000 (4.3) [a], 24300 [e], 26200 [b], 32800 [c]	24300	Very Low

Chemical	Chemical Group	Vapour pressure at 25°C unless stated (Pa)		Consensus
		Review	Recommended	
2,4,6-Trichlorophenol	Chlorophenol	1.12 (24) ^{c}, 1.25 ^{b}, 2.79 ^{e}	2.79	Very Low
α,α,α-Trichlorotoluene	Chlorotoluene	10 (9) ^{a}, 24.6 (20) ^{g}, 30.7 (20) ^{c}, 46.0 ^{b}	46.0	Low
Trifluralin	Pesticide	0.015 $^{e, f}$, 0.026 ^{b}	0.015	Low
m-Xylene	BTEX	798 (20) ^{g},1000 (23) ^{a}, 1100 ^{b}, 1110 $^{c, e}$	1110	Low
o-Xylene	BTEX	665 (20) ^{g},767 (20) ^{e}, 880 ^{c}, 1000 (27) ^{a}, 1170 ^{b}	1170	Very Low
p-Xylene	BTEX	865 (20) ^{g}, 1000 (22.4) ^{a}, 1160 ^{c}, 1170 $^{b, e}$	1170	Low

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] HOWARD, P.H., 1990. [d] MERCK, 2006. [e] MONTGOMERY, J.H., 2007. [f] MONTGOMERY, J.H., 1997. [g] OECD, 2000.

Table A9: Water solubility at specific temperature (mg L^{-1})

Chemical	Chemical Group	Water solubility at 25°C unless stated (mg L^{-1})		Consensus
		Review	Recommended	
Aldrin	Pesticide	0.020 (20) [c], 0.020 [b], 0.044 [e], 0.055 [f], 0.200 [a]	0.020	Low
Atrazine	Pesticide	12.3 (20) [e], 30 (20) [c], 30 [b], 33.8 (22) [f], 70 [a, d]	70	Low
Azinphos-methyl	Pesticide	9.5 (10) [f], 20.9 (20) [c], 20.9 (20) [a], 21 (20) [e], 30 [b], 33 [d]	9.5 (10) 20.9 (20)	Low
Benzene	BTEX	1710 [e], 1770 [g], 1780 (10) [a, g], 1780 [b], 1790 (NA) [c], 1800 [h], 1880 (24) [d]	1780 (10) 1770	High
Benzo[*a*]anthracene	PAH	3.8E-03 (10) [a], 0.011 [b, g], 0.016 [e]	3.8E-03 (10) 0.011	Low
Benzo[*b*]fluoranthene	PAH	1.2E-03 [e], 1.5E-03 [b], 2.0E-03 (20) [a]	2.0E-03 (20)	Very Low
Benzo[*k*]fluoranthene	PAH	8.0E-04 [a, b], 1.1E-03 [e]	8.0E-04	Low
Benzo[*ghi*]perylene	PAH	2.6E-04 [a, b, g], 3.1E-04 [e]	2.6E-04	Low
Benzo[*a*]pyrene	PAH	2.9E-03 [e], 3.8E-03 [b, g], 4.3E-03 [a]	3.8E-03	Low
Carbon disulphide		2100 (20) [a, c], 2100 [b], 2300 (22) [f], 2860 [e], 2940 (20) [d]	2100 (20)	Low
Chlorobenzene	Chlorobenzene	387 (10) [a], 423 [e], 454 (10) [g], 472 [c], 484 [b], 493 [g]	387 (10) 484	Low
Chloroethene		1100 [h], 1720 [e], 2700 [a], 2760 [b, c]	2760	Low
2-Chlorophenol	Chlorophenol	17800 [e], 20600 [g], 22700 [a], 24700 [b], 28000 [c]	22700	Very Low
α-Chlorotoluene	Chlorotoluene	449 (20) [b], 493 (20) [a, c], 1200 [h]	493 (20)	Low
2-Chlorotoluene	Chlorotoluene	47 (20) [h], 117 [a], 118 [e], 306 [b]	117	Low
Chrysene	PAH	7.0E-04 (7) [a], 1.9E-03 [g], 2.0E-03 [b], 2.1E-03 [e]	2.0E-03	Low
p,p'-DDT	Pesticide	2.6 E-03 [f], 5.5E-03 [b], 5.7E-03 [e]	5.7E-03	Low
o,p'-DDT	Pesticide	0.026 [b], 0.085 [e]	0.085	Very Low
Dibenz[*ah*]anthracene	PAH	5.0E-04 [a], 6.0E-04 [b, g], 1.2E-03 [e]	6.0E-04	Low
1,2-Dichlorobenzene	Chlorobenzene	94 [a], 125 [e], 133 (10) [g], 140 [b], 145 [d], 146 [g], 155.8 [h], 156 [c]	133 (10) 145	Low
1,3-Dichlorobenzene	Chlorobenzene	103 (10) [a, g], 106 [g], 111 (20) [c], 120 [b], 123 [d], 127 [e]	103 (10) 106	Low
1,4-Dichlorobenzene	Chlorobenzene	51.2 (10) [a, g], 60 (20) [h], 68 [e], 80 [b], 82.6 [g]	51.2 (10) 82.6	Low

Chemical	Chemical Group	Water solubility at 25°C unless stated (mg L^{-1})		Consensus
		Review	Recommended	
1,2-Dichloroethane		8430 [e], 8520 [c], 8600 [a, b, g], 8680 (10) [g], 8745 (20) [h]	8680 (10) 8600	High
2,4-Dichlorophenol	Chlorophenol	4400 (20) [g], 4500 [b, h], 5520 [a], 7160 [e]	4500	Low
Dichlorvos	Pesticide	8000 [b], 10000 [d], 16000 (20) [f], 16000 [c, e]	16000	Low
Dieldrin	Pesticide	0.14 (20) [f], 0.17 (20) [c], 0.17 [b], 0.20 [a, e]	0.20	Low
Endosulfan (α form)	Pesticide	0.50 [b], 0.51 (20) [c], 0.53 [e, f]	0.53	Low
Endosulfan (β form)	Pesticide	0.28 [e, f], 0.45 (20) [c], 0.45 [b]	0.28	Low
Ethylbenzene	BTEX	152 [b], 161 [a, c], 169 [g, h], 170 [e], 180 (10) [g]	180 (10) 161	Low
Fenitrothion	Pesticide	25.3 (20) [e], 30 [b]	25.3 (20)	Very Low
Fluoranthene	PAH	0.21 [a], 0.23 [e], 0.24 [g], 0.26 [b]	0.23	Low
Hexachlorobenzene	Chlorobenzene	5.0E-03 [b], 5.1E-03 [g], 6.2E-03 [c], 9.5E-03 [e], 9.6E-03 [a], 0.040 (20) [f]	9.6E-03	Low
Hexchloro-1,3-butadiene		2.6 (20) [c], 3.2 [b], 4.8 [e], 5 (20) [d], 4100 [a]	4.8	Low
α-Hexachlorocyclohexane	Pesticide	1 [b], 1.6 (20) [f], 1.8 [a], 2 [c, e]	2	Low
β-Hexachlorocyclohexane	Pesticide	0.1 [b], 0.20 [a], 0.24 [f], 0.41 [e]	0.20	Very Low
γ-Hexachlorocyclohexane	Pesticide	7.3 [b, c], 7.6 [e], 7.8 [a], 17 (24) [f]	7.3	Low
Indeno[*123-cd*]pyrene	PAH	2.0E-04 (20) [a], 2.9E-04 [b], 0.062 (NA) [e]	2.0E-04 (20)	Very Low
Malathion	Pesticide	141 (10) [f], 143 (20) [c], 144 (20) [e], 145 [b, d]	141 (10) 145	Medium
Naphthalene	PAH	19 (10) [a, g], 29.8 [e], 31 [b, g, h], 31.7 [c]	19 (10) 31	Low
Pentachlorobenzene	Chlorobenzene	0.50 [a], 0.55 [g], 0.65 [b], 0.74 [e], 1.33 [f]	0.50	Low
Pentachlorophenol	Chlorophenol	9.9 [g], 13.9 [e], 14 (20) [c, f], 14 [b], 21 [a], 80 [d]	14 (20)	Medium
Phenol		66000 [d], 81200 [e], 84000 (20) [h], 84100 [a], 87000 [c], 88400 [b]	84100	Medium
2-Propanone		441000 [e]	441000	Very Low
Pyrene	PAH	0.11 [e], 0.13 [b, g], 0.14 [a]	0.13	Low
1,2,3,4-Tetrachlorobenzene	Chlorobenzene	4.3 [g], 7.0 [a], 7.8 [b, e]	7.8	Low
1,2,3,5-Tetrachlorobenzene	Chlorobenzene	3.5 [a, g], 3.6 [b], 3.9 [e]	3.5	Low
1,2,4,5-Tetrachlorobenzene	Chlorobenzene	0.6 [a, g], 0.95 [e], 1.3 [b]	0.6	Low
1,1,1,2-Tetrachloroethane		1070 [a, b, g], 1100 [c], 1110 (10) [g]	1110 (10) 1070	Medium
1,1,2,2-Tetrachloroethane		2830 [a, b, g], 2850 [d], 2870 (20) [h], 2930 (10) [g], 2940 [e], 2960 [c]	2930 (10) 2830	Medium

Chemical	Chemical Group	Water solubility at 25°C unless stated (mg L^{-1})		Consensus
		Review	Recommended	
Tetrachloroethene		150 [b, c], 206 [g], 210 (20) [a], 225 (10) [g], 270 [e]	225 (10) 150	Low
Tetrachloromethane		650 [a], 782 [e], 800 (20) [f], 800 [b], 805 (20) [c], 813 [g], 846 (10) [g]	846 (10) 800	Medium
2,3,4,6-Tetrachlorophenol	Chlorophenol	0.174 [e], 170 [a], 183 [b, g]	183	Low
Tetraethyl lead		0.155 [e]	0.155	Very Low
Toluene	BTEX	515 [b], 515 (20) [h], 519 [a], 522 [e], 530 [g], 535 [c], 590 (10) [g]	590 (10) 522	Medium
Tributyl tin oxide (TBTO)			none	
1,2,3-Trichlorobenzene	Chlorobenzene	17.8 [e], 21 [a, b], 30.8 [g]	21	Low
1,2,4-Trichlorobenzene	Chlorobenzene	35.3 (20) [h], 37 [a], 40 [b], 41.4 [e], 48.8 (20) [c], 553 [g]	41.4	Low
1,3,5-Trichlorobenzene	Chlorobenzene	2.8 [e], 5.3 [b], 6 [c], 6.5 [g], 8 [a]	6	Very Low
1,1,1-Trichloroethane		680 [e], 1290 [a, b, g], 1300 (10) [g], 1500 [c]	1300 (10) 1290	Medium
Trichloroethene		1000 (20) [h], 1100 [b, c, d], 1270 [e], 1280 [a, g], 1370 (10) [g]	1370 (10) 1100	Low
Trichloromethane		7820 [e], 7950 (NA) [c], 7980 [g], 8000 [a], 8200 [b], 8950 (10) [g]	8950 (10) 7980	Medium
2,4,6-Trichlorophenol	Chlorophenol	434 [b, g], 604 [e], 692 [a], 900 [c]	434	Low
α,α,α-Trichlorotoluene	Chlorotoluene	5.3 (5) [b], 52.6 (5) [e], 100 (20) [h]	52.6 (5)	Very Low
Trifluralin	Pesticide	0.24 [d], 0.5 [b], 1 [e], 4 (27) [f]	1	Very Low
m-Xylene	BTEX	146 [c], 160 [b, g], 161 [a, h], 162 [e], 200 (10) [g]	200 (10) 161	Medium
o-Xylene	BTEX	171 [a], 173 [g], 175 [c], 178 [h], 192 [e], 220 [b]	173	Low
p-Xylene	BTEX	156 [c], 162 [h], 180 [g], 181 [a], 185 [e], 200 (10) [g], 215 [b]	200 (10) 181	Low

Notes

[a] LIDE, D.R., 2008. [b] MACKAY, D., SHIU, W-Y., MA, K-C., LEE, S., 2006. [c] HOWARD, P.H., 1990. [d] MERCK, 2006. [e] MONTGOMERY, J.H., 2007. [f] MONTGOMERY, J.H., 1997. [g] IUPAC-NIST (2006). [h] OECD, 2000.

Appendix B

Comparison of methods for estimating the Henry's law constant of a chemical with recommended literature values and the calculated values of the air-water partition coefficient for use in the derivation of Soil Guideline Values (see 2.1.3 and 2.1.4 for further information)

Table B1: Air-water partition coefficients at 10°C by direct calculation (dimensionless)

Chemical	Water solubility at 10°C (mol m^{-3})	Vapour pressure at 10°C (Pa)	Air-water partition coefficients at 10°C (dimensionless)
Azinphos methyl	2.99E-02	2.37E-09	3.36E-11
Benzene	2.28E+01	6.24E+03	1.16E-01
Benz[a]anthracene	1.66E-05	1.24E-06	3.16E-05
Chlorobenzene	3.44E+00	6.73E+02	8.31E-02
1,2-Dichlorobenzene	9.05E-01	7.21E+01	3.38E-02
1,3-Dichlorobenzene	7.01E-01	1.09E+02	6.61E-02
1,4-Dichlorobenzene	3.48E-01	3.85E+01	4.70E-02
1,2-Dichloroethane	8.77E+01	4.92E+03	2.38E-02
Ethylbenzene	1.70E+00	5.53E+02	1.39E-01
Malathion	4.27E-01	9.22E-04	9.18E-07
Naphthalene	1.48E-01	2.31E+00	6.62E-03
1,1,1,2-Tetrachloroethane	6.61E+00	7.48E+02	4.80E-02
1,1,2,2-Tetrachloroethane	1.75E+01	2.91E+02	7.08E-03
Tetrachloroethene	1.36E+00	1.01E+03	3.16E-01
Tetrachloromethane	5.50E+00	7.53E+03	5.82E-01
Toluene	6.40E+00	1.73E+03	1.15E-01
1,1,1-Trichloroethane	9.75E+00	8.25E+03	3.60E-01
Trichloroethene	1.04E+01	4.58E+03	1.87E-01
Trichloromethane	7.50E+01	1.35E+04	7.65E-02
m-Xylene	1.88E+00	4.95E+02	1.12E-01
p-Xylene	1.88E+00	4.75E+02	1.07E-01

Table B2: Comparison of estimated and literature values for the Henry's Law constant at 25°C (Pa m^3 mol^{-1})

Chemical	Henry's Law constant (Pa m^3 mol^{-1}) at 20 or 25°C			Absolute error (per cent or order of magnitude)	
	Literature [1]	Direct calculation	Meylan and Howard [2]	Direct Calculation	Meylan and Howard
Aldrin	5.03E+01	9.12E+01	3.92E+01 [b]	same order	22.0
Atrazine	2.88E-04	1.23E-04	4.53E-04 [b]	same order	same order
Azinphos-methyl	3.17E-04		2.90E-05 [b]		one order
Benzene	5.57E+02	5.60E+02	5.46E+02 [b]	0.6	1.9
Benzo[*a*]anthracene	5.80E-01	5.81E-01	5.08E-01 [b]	0.2	12.5
Benzo[*b*]fluoranthene	5.10E-02	8.41E+00	5.44E-01 [b]	two orders	one order
Benzo[*k*]fluoranthene	4.30E-02	4.04E-03	1.63E-01 [b]	one order	same order
Benzo[*ghi*]perylene	7.50E-02	1.52E-02	1.33E-02 [b]	same order	same order
Benzo[*a*]pyrene	4.60E-02	2.03E-01	2.06E-02 [g]	one order	same order
Carbon disulphide	1.75E+03	1.74E+03	3.06E+03 [b]	0.6	same order
Chlorobenzene	3.67E+02	3.67E+02	4.04E+02 [b]	0.1	10.2
Chloroethene	2.69E+03	8.04E+03	4.50E+03 [b]	same order	same order
2-Chlorophenol	6.53E-01	1.35E+00	5.67E-02 [g]	one order	one order
α-Chlorotoluene	3.60E+01	4.44E+01	4.02E+01 [g]	23.4	11.7
2-Chlorotoluene	2.95E+02	5.17E+02	4.47E+02 [b]	same order	same order
Chrysene	6.50E-02	7.91E-02	1.79E-01 [g]	21.7	same order
p,*p*'-DDT	9.03E-01	1.24E+00	1.55E+00 [b]	37.7	same order
Dibenz[*ah*]anthracene	1.72E-01	1.72E-04	4.95E-02 [b]	three orders	same order
1,2-Dichlorobenzene	1.95E+02	1.99E+02	3.00E+02 [b]	1.9	same order
1,3-Dichlorobenzene	3.18E+02	3.90E+02	3.00E+02 [b]	22.5	5.7
1,4-Dichlorobenzene	2.44E+02	1.26E+02	3.00E+02 [b]	48.4	22.9
1,2-Dichloroethane	1.21E+02	1.21E+02	1.97E+01 [g]	0.1	one order
2,4-Dichlorophenol	3.27E-01	4.31E-01	4.83E-02 [g]	31.8	one order
Dichlorvos	5.59E-03	9.71E-02	8.69E-02 [b]	one order	one order
Dieldrin	5.88E+00	9.52E-01	5.48E-02 [b]	same order	two orders
Endosulfan (α form)	7.68E+00	4.69E+00	9.15E-03 [b]	38.9	three orders
Endosulfan (β form)	5.12E+00	4.65E+00	9.15E-03 [b]	9.2	three orders
Ethylbenzene	8.43E+02	8.37E+02	7.99E+02 [b]	0.7	5.2
Fenitrothion	9.50E-02	8.77E-03	1.88E-02 [b]	one order	one order
Fluoranthene	9.60E-01	2.75E+00	1.67E+00 [b]	one order	same order
Hexachlorobenzene	1.31E+02	4.30E+01	9.04E+01 [b]	same order	31.0
Hexchloro-1,3-butadiene	1.03E+03	1.09E+03	1.09E+03 [b]	5.5	6.2

Chemical	Henry's Law constant (Pa m^3 mol^{-1}) at 20 or 25°C			Absolute error (per cent or order of magnitude)	
	Literature [1]	Direct calculation	Meylan and Howard [2]	Direct Calculation	Meylan and Howard
α-Hexachlorocyclohexane	8.72E-01	3.36E+01	2.59E+01 [b]	two orders	one order
β-Hexachlorocyclohexane	4.50E-02	9.03E-02	2.59E+01 [b]	same order	three orders
γ-Hexachlorocyclohexane	3.75E-01	4.98E-02	2.59E+01 [b]	one order	two orders
Indeno[*123-cd*]pyrene	2.90E-02	1.87E-02	2.01E-01 [b]	35.7	one order
Malathion	4.95E-04	2.28E-03	8.50E-05 [b]	one order	one order
Naphthalene	4.30E+01	4.30E+01	3.75E+01 [g]	0.0	12.8
Pentachlorobenzene	8.50E+01	1.10E+02	1.22E+02 [b]	29.6	43.0
Pentachlorophenol	7.90E-02	6.66E-01	2.98E-02 [g]	one order	same order
Phenol	6.50E-02	6.26E-02	6.67E-02 [g]	3.8	2.6
2-Propanone	3.76E+00	4.06E+00	4.02E+00 [g]	7.9	7.0
Pyrene	9.20E-01	2.57E+00	8.41E-01 [b]	same order	8.6
1,2,3,4-Tetrachlorobenzene	1.44E+02	8.39E+01	1.64E+02 [b]	41.8	14.0
1,2,3,5-Tetrachlorobenzene	5.88E+02	5.33E+02	2.85E+02 [g]	9.4	same order
1,2,4,5-Tetrachlorobenzene	1.22E+02	2.40E+02	1.64E+02 [b]	same order	34.5
1,1,1,2-Tetrachloroethane	2.45E+02	2.48E+02	1.53E+02 [b]	1.2	37.6
1,1,2,2-Tetrachloroethane	4.61E+01	4.70E+01	1.53E+02 [b]	2.0	same order
Tetrachloroethene	1.73E+03	2.73E+03	1.67E+03 [b]	57.8	3.4
Tetrachloromethane	2.99E+03	2.94E+03	3.04E+03 [g]	1.6	1.7
2,3,4,6-Tetrachlorophenol	3.55E-01	3.55E-01	3.51E-02 [g]	0.1	one order
Toluene	6.60E+02	6.69E+02	6.03E+02 [b]	1.4	8.7
1,2,3-Trichlorobenzene	2.42E+02	6.25E+02	2.22E+02 [b]	same order	8.3
1,2,4-Trichlorobenzene	2.77E+02	1.75E+02	2.22E+02 [b]	36.7	19.9
1,3,5-Trichlorobenzene	1.10E+03	2.34E+03	3.34E+02 [g]	same order	one order
1,1,1-Trichloroethane	1.71E+03	1.71E+03	1.64E+03 [g]	0.2	4.0
Trichloroethene	1.03E+03	1.17E+03	1.88E+03 [g]	13.3	same order
Trichloromethane	4.30E+02	3.64E+02	4.11E+02 [g]	15.5	4.3
2,4,6-Trichlorophenol	9.19E-03	1.27E+00	2.31E-02 [b]	three orders	same order
Trifluralin	5.91E+00	5.03E+00	2.15E+01 [b]	14.9	same order
m-Xylene	7.30E+02	7.32E+02	6.65E+02 [b]	0.3	8.9
o-Xylene	5.51E+02	7.18E+02	6.22E+02 [g]	30.3	20.6
p-Xylene	6.69E+02	6.86E+02	6.65E+02 [b]	2.6	0.6

[1] See recommended values in Table A4.

[2] Meylan and Howard (1991) use two estimation techniques; the most accurate is reported for each chemical.

[b] indicates the bond contribution method and [g] indicates the group contribution method.

Table B3: Air-water partition coefficients at 10°C (dimensionless)

Chemical	Air-water partition coefficients at 10°C unless otherwise stated (dimensionless) [a]
Aldrin	5.79E-03
Atrazine	2.81E-08
Azinphos-methyl	3.36E-11 [†]
Benzene	1.16E-01 [†]
Benzo[*a*]anthracene	3.16E-05 [†]
Benzo[*b*]fluoranthene	2.05E-06
Benzo[*k*]fluoranthene	1.74E-06
Benzo[*ghi*]perylene	2.36E-06
Benzo[*a*]pyrene	1.76E-06
Carbon disulphide	4.08E-01
Chlorobenzene	8.31E-02 [†]
Chloroethene	7.47E-01
2-Chlorophenol	1.35E-04
α-Chlorotoluene	7.47E-03 [‡]
2-Chlorotoluene	6.47E-02 [‡]
Chrysene	3.18E-06
p,*p*'-DDT	8.17E-05
Dibenz[*ah*]anthracene	5.40E-06
1,2-Dichlorobenzene	3.38E-02 [†]
1,3-Dichlorobenzene	6.61E-02 [†]
1,4-Dichlorobenzene	4.70E-02 [†]
1,2-Dichloroethane	2.38E-02 [†]
2,4-Dichlorophenol	5.07E-05
Dichlorvos	6.51E-07
Dieldrin	2.73E-04
Endosulfan (α form)	1.89E-03 (25°C) [†]
Endosulfan (β form)	1.88E-03 (25°C) [†]
Ethylbenzene	1.39E-01 [†]
Fenitrothion	3.60E-06 (20°C) [†]
Fluoranthene	6.29E-05
Hexachlorobenzene	1.04E-02
Hexchloro-1,3-butadiene	1.55E-01
α-Hexachlorocyclohexane	8.11E-05
β-Hexachlorocyclohexane	4.71E-06

Chemical	Air-water partition coefficients at 10°C unless otherwise stated (dimensionless) [a]
γ-Hexachlorocyclohexane	3.10E-05
Indeno[*123-cd*]pyrene	2.05E-06 [‡]
Malathion	9.18E-07 [†]
Naphthalene	6.62E-03 [†]
Pentachlorobenzene	8.30E-03
Pentachlorophenol	5.55E-06
Phenol	8.35E-06
2-Propanone	8.11E-04
Pyrene	5.64E-05
1,2,3,4-Tetrachlorobenzene	1.58E-02
1,2,3,5-Tetrachlorobenzene	6.61E-02
1,2,4,5-Tetrachlorobenzene	1.38E-02
1,1,1,2-Tetrachloroethane	4.80E-02 [†]
1,1,2,2-Tetrachloroethane	7.08E-03 [†]
Tetrachloroethene	3.16E-01 [†]
Tetrachloromethane	5.82E-01 [†]
2,3,4,6-Tetrachlorophenol	3.96E-05
Tetraethyl lead	6.20E-02
Toluene	1.15E-01 [†]
Tributyl tin oxide (TBTO)	4.24E-05
1,2,3-Trichlorobenzene	3.07E-02
1,2,4-Trichlorobenzene	3.65E-02
1,3,5-Trichlorobenzene	1.44E-01
1,1,1-Trichloroethane	3.60E-01 [†]
Trichloroethene	1.87E-01 [†]
Trichloromethane	7.65E-02 [†]
2,4,6-Trichlorophenol	8.82E-07
α,α,α-Trichlorotoluene	3.20E-03
Trifluralin	2.87E-04 [‡]
m-Xylene	1.12E-01 [†]
o-Xylene	9.20E-02
p-Xylene	1.07E-01 [†]

[a] Estimated by temperature adjustment of Henry's Law constant using the Clapeyron equation.

[‡] Indicates that the Henry's Law constant used in the calculation was measured at either 20 or 23°C

[†] K_{aw} calculated from direct measurement of vapour pressure & water solubility at 10°C or other temp.

Appendix C

Comparison between the methods for estimating the normal boiling point of a chemical and the recommended literature values

Table C1: Normal boiling point (K)

Chemical	Normal boiling point (K)			Absolute error (per cent)	
	Literature value [a]	Banks' Method	MP Correlation [b]	Banks' Method	MP Correlation
Benzene	353.2	336.8	366.6	4.6	3.8
Benz[a]anthracene	711.2	519.1	686.6	27.0	3.5
Benzo[b]fluoranthene	754.2	534.8	722.0	29.1	4.3
Benzo[k]fluoranthene	753.2	534.8	732.7	29.0	2.7
Benzo[ghi]perylene	798.2	548.7	792.6	31.3	0.7
Benzo[a]pyrene	768.2	534.8	728.7	30.4	5.1
Carbon disulphide	319.2	332.3	280.5	4.1	12.1
Chlorobenzene	404.9	400.8	393.4	1.0	2.8
Chloroethene	259.4	297.9	289.3	14.8	11.5
2-Chlorophenol	448.1	423.9	464.0	5.4	3.6
α-Chlorotoluene	452.2	421.2	423.8	6.9	6.3
2-Chlorotoluene	432.2	421.2	428.5	2.5	0.9
Chrysene	721.2	519.1	720.7	28.0	0.1
DDT (p,p'-)	533.2	585.5	675.9	9.8	26.8
Dibenz[ah]anthracene	797.2	549.9	791.0	31.0	0.8
1,2-Dichlorobenzene	453.7	446.8	423.7	1.5	6.6
1,3-Dichlorobenzene	446.2	446.8	419.8	0.1	5.9
1,4-Dichlorobenzene	447.2	446.8	445.1	0.1	0.5
1,2-Dichloroethane	356.7	378.4	365.3	6.1	2.4
2,4-Dichlorophenol	483.2	464.2	498.0	3.9	3.1
Dichlorvos	507.2	513.9	-	1.3	-
Ethylbenzene	409.4	390.7	398.3	4.6	2.7
Fluoranthene	657.2	499.7	615.0	24.0	6.4
Hexachlorobenzene	597.7	553.3	575.3	7.4	3.8
Hexachloro-1,3-butadiene	488.2	539.9	453.3	10.6	7.2
α-Hexachlorocyclohexane	561.2	556.5	576.2	0.8	2.7
γ-Hexachlorocyclohexane	596.6	556.5	553.0	6.7	7.3
Indeno[123-cd]pyrene	809.2	548.7	750.6	32.2	7.2

Chemical	Normal boiling point (K)			Absolute error (per cent)	
	Literature value [a]	Banks' Method	MP Correlation [b]	Banks' Method	MP Correlation
Naphthalene	491.1	423.3	490.6	13.8	0.1
Pentachlorobenzene	550.2	533.6	523.7	3.0	4.8
Pentachlorophenol	583.2	543.1	596.8	6.9	2.3
Phenol	455.0	369.5	449.9	18.8	1.1
2-Propanone	329.3	285.2	320.9	13.4	2.5
Pyrene	677.2	499.7	621.3	26.2	8.3
1,2,3,4-Tetrachlorobenzene	527.2	510.2	488.2	3.2	7.4
1,2,3,5-Tetrachlorobenzene	519.2	510.2	491.8	1.7	5.3
1,2,4,5-Tetrachlorobenzene	517.7	510.2	520.8	1.4	0.6
1,1,1,2-Tetrachloroethane	403.4	469.1	379.3	16.3	6.0
1,1,2,2-Tetrachloroethane	419.7	469.1	379.2	11.8	9.7
Tetrachloroethene	394.5	467.1	375.1	18.4	4.9
Tetrachloromethane	350.0	454.4	336.2	29.8	3.9
Tetraethyl lead	473.2	572.2	-	20.9	-
Toluene	383.8	365.8	368.2	4.7	4.1
1,2,3-Trichlorobenzene	491.7	482.0	474.4	2.0	3.5
1,2,4-Trichlorobenzene	486.7	482.0	471.2	1.0	3.2
1,3,5-Trichlorobenzene	481.2	482.0	457.5	0.2	4.9
1,1,1-Trichloroethane	347.2	430.2	361.3	23.9	4.1
Trichloroethene	360.4	427.6	356.1	18.6	1.2
Trichloromethane	334.3	411.1	328.4	23.0	1.8
2,4,6-Trichlorophenol	519.2	495.8	511.7	4.5	1.4
α,α,α-Trichlorotoluene	494.2	494.2	476.0	0.0	3.7
Trifluralin	635.2	577.5	661.3	9.1	4.1
m-Xylene	412.5	390.7	408.0	5.3	1.1
o-Xylene	417.6	390.7	419.6	6.5	0.5
p-Xylene	411.5	390.7	424.8	5.1	3.2

Average	11.7	4.4

Notes

[a] see recommended values in Table A1

[b] see recommended values in Table A5

Appendix D

Comparison between the methods for estimating the critical point temperature of a chemical and recommended literature values

Table D1: Critical point temperature (K)

Chemical	**Critical point temperature (K)**			**Absolute error (per cent)**	
	Literature value	**Guldberg approx.**	**Lydersen method**	**Guldberg approx.**	**Lydersen method**
Benzene	562.0	530.0	562.0	5.7	0.0
Carbon disulphide	552.0	478.8	557.1	13.3	0.9
Chlorobenzene	633.4	607.4	629.6	4.1	0.6
Chloroethene	432.0	389.1	420.3	9.9	2.7
1,3-Dichlorobenzene	685.7	669.3	679.1	2.4	1.0
1,2-Dichloroethane	561.0	535.1	561.3	4.6	0.0
Ethylbenzene	617.2	614.1	618.6	0.5	0.2
Naphthalene	748.4	736.7	738.6	1.6	1.3
Phenol	694.2	682.5	695.1	1.7	0.1
2-Propanone	508.1	494.0	514.0	2.8	1.2
1,1,2,2-Tetrachloroethane	661.2	629.6	645.2	4.8	2.4
Tetrachloroethene	620.2	591.8	625.8	4.6	0.9
Tetrachloromethane	556.6	525.0	555.2	5.7	0.2
Toluene	591.8	575.7	594.5	2.7	0.5
1,2,4-Trichlorobenzene	730.7	730.1	726.1	0.1	0.6
1,1,1-Trichloroethane	545.0	520.8	548.5	4.4	0.6
Trichloroethene	544.2	540.6	570.9	0.7	4.9
Trichloromethane	536.4	501.5	534.0	6.5	0.4
m-Xylene	617.0	618.8	623.3	0.3	1.0
o-Xylene	630.3	626.4	631.0	0.6	0.1
p-Xylene	616.2	617.3	621.8	0.2	0.9
			Average	3.7	1.0

Notes

[a] see recommended values in Table A2

[b] derived using structural increment table in Lyman *et al.* 1990

Appendix E

Calculated values for the coefficient of diffusion in air (see 2.4.4 for further information)

Table E1: Diffusion coefficients in air at 10°C ($m^2 s^{-1}$)

Chemical	Molar Volume	Coefficient of diffusion in air ($m^2 s^{-1}$)	
	$cm^3 mol^{-1}$	FSG method	WL method
Aldrin	316.8	4.15E-06	4.12 E-06 [b]
Atrazine	250.6	4.75 E-06	4.69 E-06 [b]
Azinphos-methyl	270.4	4.50 E-06	4.40 E-06 [b]
Benzene	96.0	7.98 E-06	8.77 E-06
Benzo[*a*]anthracene	248.3	4.75 E-06	4.60 E-06
Benzo[*b*]fluoranthene	268.9	4.56 E-06	4.36 E-06
Benzo[*k*]fluoranthene	268.9	4.56 E-06	4.36 E-06
Benzo[*ghi*]perylene	277.5	4.47 E-06	4.22 E-06
Benzo[*a*]pyrene	262.9	4.60 E-06	4.38 E-06
Carbon disulphide	66.0	9.34 E-06	1.04 E-05
Chlorobenzene	116.9	7.03 E-06	7.57 E-06
Chloroethene	65.3	9.65 E-06	1.11 E-05
2-Chlorophenol	124.3	6.76 E-06	7.14 E-06
α-Chlorotoluene	139.1	6.45 E-06	6.81 E-06
2-Chlorotoluene	139.1	6.45 E-06	6.88 E-06
Chrysene	250.8	4.73 E-06	4.57 E-06
p,*p*'-DDT	333.5	4.05 E-06	4.22 E-06
Dibenz[*ah*]anthracene	299.9	4.31 E-06	4.08 E-06
1,2-Dichlorobenzene	137.8	6.39 E-06	6.75 E-06
1,3-Dichlorobenzene	137.8	6.39 E-06	6.77 E-06
1,4-Dichlorobenzene	137.8	6.39 E-06	6.77 E-06
1,2-Dichloroethane	93.6	7.83 E-06	8.60 E-06
2,4-Dichlorophenol	145.2	6.20 E-06	6.46 E-06
Dichlorvos	167.5	5.70 E-06	5.91 E-06
Dieldrin	318.2	4.13 E-06	4.03 E-06 [b]
Endosulfan (α form)	312.8	4.16 E-06	4.08 E-06 [b]
Endosulfan (β form)	312.8	4.16 E-06	4.01 E-06 [b]
Ethylbenzene	140.4	6.54 E-06	7.04 E-06
Fenitrothion	229.7	4.88 E-06	4.90 E-06 [b]

Chemical	Molar Volume	Coefficient of diffusion in air ($m^2 s^{-1}$)	
	$cm^3 mol^{-1}$	FSG method	WL method
Fluoranthene	217.3	5.09 E-06	5.01 E-06
Hexachlorobenzene	221.4	4.96 E-06	4.99 E-06
Hexchloro-1,3-butadiene	206.8	5.14 E-06	5.40 E-06
α-Hexachlorocyclohexane	243.6	4.74 E-06	4.84 E-06
β-Hexachlorocyclohexane	243.6	4.74 E-06	4.72 E-06 [b]
γ-Hexachlorocyclohexane	243.6	4.74 E-06	4.78 E-06
Indeno[*123-cd*]pyrene	283.5	4.42 E-06	4.17 E-06
Malathion	319.1	4.15 E-06	4.12 E-06 [b]
Naphthalene	147.6	6.28 E-06	6.52 E-06
Pentachlorobenzene	200.5	5.22 E-06	5.34 E-06
Pentachlorophenol	207.9	5.12 E-06	5.17 E-06
Phenol	103.4	7.56 E-06	7.90 E-06
2-Propanone	74.0	9.29 E-06	1.03 E-05
Pyrene	213.8	5.13 E-06	5.01 E-06
1,2,3,4-Tetrachlorobenzene	179.6	5.53 E-06	5.69 E-06
1,2,3,5-Tetrachlorobenzene	179.6	5.53 E-06	5.71 E-06
1,2,4,5-Tetrachlorobenzene	179.6	5.53 E-06	5.72 E-06
1,1,1,2-Tetrachloroethane	135.4	6.37 E-06	6.90 E-06
1,1,2,2-Tetrachloroethane	135.4	6.37 E-06	6.84 E-06
Tetrachloroethene	128.0	6.54 E-06	7.10 E-06
Tetrachloromethane	113.2	6.93 E-06	7.69 E-06
2,3,4,6-Tetrachlorophenol	187.0	5.41 E-06	5.54 E-06 [b]
Tetraethyl lead	195.7 [a]	5.22 E-06	5.51 E-06
Toluene	118.2	7.16 E-06	7.78 E-06
Tributyl tin oxide (TBTO)	509.5 [a]	3.24 E-06	3.25 E-06 [b]
1,2,3-Trichlorobenzene	158.7	5.91 E-06	6.16 E-06
1,2,4-Trichlorobenzene	158.7	5.91 E-06	6.17 E-06
1,3,5-Trichlorobenzene	158.7	5.91 E-06	6.19 E-06
1,1,1-Trichloroethane	114.5	6.98 E-06	7.75 E-06
Trichloroethene	107.1	7.19 E-06	7.91 E-06
Trichloromethane	92.3	7.73 E-06	8.60 E-06
2,4,6-Trichlorophenol	166.1	5.76 E-06	5.94 E-06
α,α,α-Trichlorotoluene	180.9	5.55 E-06	5.79 E-06
Trifluralin	295.9	4.30 E-06	4.29 E-06
m-Xylene	140.4	6.54 E-06	7.03 E-06

Chemical	Molar Volume	Coefficient of diffusion in air ($m^2 s^{-1}$)	
	$cm^3 mol^{-1}$	FSG method	WL method
o-Xylene	140.4	6.54 E-06	7.01 E-06
p-Xylene	140.4	6.54 E-06	7.04 E-06

Notes

[a] Molar volume estimated from liquid density at 20°C

[b] Based on estimated boiling point (see individual chemical profile in Chapter 3)

Appendix F

Comparison of calculated values for the coefficient of diffusion in water with literature data and the recommended values for use in the derivation of Soil Guideline Values (see 2.5.4 for further information)

Table F1: Comparison of experimental and calculated diffusion coefficients in water ($m^2 s^{-1}$)

Chemical	Coefficient of diffusion in water at specified temperature in °C		Absolute Difference
	Experimental [a]	Hayduk and Laudie method	
	$m^2 s^{-1}$	$m^2 s^{-1}$	%
Benzene	1.10 E-09 (25)	1.03 E-09 (25)	6.4
Benzo[*a*]anthracene	3.35 E-10 (25)	5.88 E-10 (25)	75.5
Chlorobenzene	1.00 E-09 (25)	9.16 E-10 (25)	8.4
2-Chlorophenol	9.20 E-10 (25)	8.84 E-10 (25)	3.9
1,2-Dichlorobenzene	9.40 E-10 (25)	8.32 E-10 (25)	11.5
1,4-Dichlorobenzene	9.90 E-10 (25)	8.32 E-10 (25)	16.0
Ethylbenzene	8.10 E-10 (20)	7.19 E-10 (20)	11.2
Naphthalene	7.49 E-10 (25)	7.99 E-10 (25)	6.6
Phenol	9.98 E-10 (25)	9.85 E-10 (25)	1.3
2-Propanone	1.21 E-09 (25)	1.20 E-09 (25)	0.9
Toluene	9.32 E-10 (25)	9.10 E-10 (25)	2.3
o-Xylene	7.00 E-10 (25)	8.23 E-10 (25)	17.5

Notes

[a] Experimental data reported by Montgomery (2007) at specified temperature

Table F2: Diffusion coefficients in water at 10°C ($m^2 s^{-1}$)

Chemical	Molar Volume	Coefficient of diffusion in water ($m^2 s^{-1}$)
	$cm^3 mol^{-1}$	Hayduk and Laudie method
Aldrin	316.8	3.29 E-10
Atrazine	250.6	3.78 E-10
Azinphos-methyl	270.4	3.61 E-10
Benzene	96.0	6.64 E-10
Benzo[*a*]anthracene	248.3	3.80 E-10
Benzo[*b*]fluoranthene	268.9	3.62 E-10

Chemical	Molar Volume	Coefficient of diffusion in water (m^2 s^{-1})
	cm^3 mol^{-1}	Hayduk and Laudie method
Benzo[*k*]fluoranthene	268.9	3.62 E-10
Benzo[*ghi*]perylene	277.5	3.56 E-10
Benzo[*a*]pyrene	262.9	3.67 E-10
Carbon disulphide	66.0	8.28 E-10
Chlorobenzene	116.9	5.92 E-10
Chloroethene	65.3	8.34 E-10
2-Chlorophenol	124.3	5.71 E-10
α-Chlorotoluene	139.1	5.34 E-10
2-Chlorotoluene	139.1	5.34 E-10
Chrysene	250.8	3.77 E-10
p,p'-DDT	333.5	3.19 E-10
Dibenz[*ah*]anthracene	299.9	3.40 E-10
1,2-Dichlorobenzene	137.8	5.37 E-10
1,3-Dichlorobenzene	137.8	5.37 E-10
1,4-Dichlorobenzene	137.8	5.37 E-10
1,2-Dichloroethane	93.6	6.74 E-10
2,4-Dichlorophenol	145.2	5.21 E-10
Dichlorvos	167.5	4.79 E-10
Dieldrin	318.2	3.28 E-10
Endosulfan (α form)	312.8	3.31 E-10
Endosulfan (β form)	312.8	3.31 E-10
Ethylbenzene	140.4	5.31 E-10
Fenitrothion	229.7	3.97 E-10
Fluoranthene	217.3	4.11 E-10
Hexachlorobenzene	221.4	4.06 E-10
Hexchloro-1,3-butadiene	206.8	4.23 E-10
α-Hexachlorocyclohexane	243.6	3.84 E-10
β-Hexachlorocyclohexane	243.6	3.84 E-10
γ-Hexachlorocyclohexane	243.6	3.84 E-10
Indeno[*123-cd*]pyrene	283.5	3.51 E-10
Malathion	319.1	3.27 E-10
Naphthalene	147.6	5.16 E-10
Pentachlorobenzene	200.5	4.31 E-10
Pentachlorophenol	207.9	4.21 E-10
Phenol	103.4	6.36 E-10

Chemical	Molar Volume	Coefficient of diffusion in water (m^2 s^{-1})
	cm^3 mol^{-1}	Hayduk and Laudie method
2-Propanone	74.0	7.74 E-10
Pyrene	213.8	4.15 E-10
1,2,3,4-Tetrachlorobenzene	179.6	4.59 E-10
1,2,3,5-Tetrachlorobenzene	179.6	4.59 E-10
1,2,4,5-Tetrachlorobenzene	179.6	4.59 E-10
1,1,1,2-Tetrachloroethane	135.4	5.43 E-10
1,1,2,2-Tetrachloroethane	135.4	5.43 E-10
Tetrachloroethene	128.0	5.61 E-10
Tetrachloromethane	113.2	6.03 E-10
2,3,4,6-Tetrachlorophenol	187.0	4.49 E-10
Tetraethyl lead	195.7 [a]	4.37 E-10
Toluene	118.2	5.88 E-10
Tributyl tin oxide (TBTO)	509.5 [a]	2.49 E-10
1,2,3-Trichlorobenzene	158.7	4.94 E-10
1,2,4-Trichlorobenzene	158.7	4.94 E-10
1,3,5-Trichlorobenzene	158.7	4.94 E-10
1,1,1-Trichloroethane	114.5	5.99 E-10
Trichloroethene	107.1	6.23 E-10
Trichloromethane	92.3	6.80 E-10
2,4,6-Trichlorophenol	166.1	4.81 E-10
α,α,α-Trichlorotoluene	180.9	4.57 E-10
Trifluralin	295.9	3.42 E-10
m-Xylene	140.4	5.31 E-10
o-Xylene	140.4	5.31 E-10
p-Xylene	140.4	5.31 E-10

Notes

[a] Molar volume estimated from liquid density at 20°C

Appendix G

Comparison between the methods for estimating the enthalpy of vapourisation of a chemical at normal boiling point and recommended literature values

Table G1: Enthalpy of vapourisation at normal boiling point (J mol^{-1})

Chemical	Enthalpy of vapourisation at normal boiling point (J mol^{-1})			Absolute error (per cent)	
	Literature value	Fishtine method	Modified Klein method	Fishtine method	Modified Klein method
Azinphos-methyl	96650	66490	-	31.2	-
Benzene	30720	30173	30775	1.8	0.2
Carbon disulphide	26740	27270	27244	2.0	1.9
Chlorobenzene	35190	36234	35474	3.0	0.8
Chloroethene	20800	22354	21652	7.5	4.1
2-Chlorophenol	40050	45041	44955	12.5	12.2
2-Chlorotoluene	37500	38821	38407	3.5	2.4
1,2-Dichlorobenzene	39660	41688	40655	5.1	2.5
1,3-Dichlorobenzene	38620	40326	39214	4.4	1.5
1,4-Dichlorobenzene	38790	39080	40074	0.7	3.3
1,2-Dichloroethane	31980	32026	31607	0.1	1.2
2,4-Dichlorophenol	36780	48918	48575	33.0	32.1
Dieldrin	76600	-	47977	-	37.4
Ethylbenzene	35570	35895	36004	0.9	1.2
Naphthalene	43200	43307	42336	0.2	2.0
Phenol	45690	45801	45733	0.2	0.1
2-Propanone	29100	30174	30512	3.7	4.9
1,1,1,2-Tetrachloroethane	34780	36652	34835	5.4	0.2
1,1,2,2-Tetrachloroethane	37640	38278	35078	1.7	6.8
Tetrachloroethene	34680	34404	33227	0.8	4.2
Tetrachloromethane	29820	30172	29951	1.2	0.4
Tetraethyl lead	56600	41159		27.3	
Toluene	33180	33300	33738	0.4	1.7
1,1,1-Trichloroethane	29860	31091	30085	4.1	0.8
Trichloroethene	31400	32391	34071	3.2	8.5
Trichloromethane	29240	29826	29285	2.0	0.2
m-Xylene	35660	36129	36896	1.3	3.5

Chemical	Enthalpy of vapourisation at normal boiling point (J mol^{-1})			Absolute error (per cent)	
	Literature value	Fishtine method	Modified Klein method	Fishtine method	Modified Klein method
o-Xylene	36240	36720	36634	1.3	1.1
p-Xylene	35670	35676	36716	0.0	2.9

Average	5.7	5.1

Appendix H

Comparison between the methods for estimating the octanol-water coefficient of a chemical and recommended literature values (see 2.7.4 for further details)

Table H1: Comparison of measured and estimated values of the logarithm of the octanol-water partition coefficient (dimensionless)

Chemical	log K_{ow} (dimensionless)			Absolute error (per cent)	
	Literature	KOWWIN	CLOGP	KOWWIN	CLOGP
Aldrin	6.47	6.75	6.45	4.3	0.3
Atrazine	2.75	2.82	2.70	2.5	1.8
Azinphos-methyl	2.69	2.53	2.55	5.9	5.2
Benzene	2.13	1.99	2.14	6.6	0.5
Benzo[*a*]anthracene	5.91	5.52	5.66	6.6	4.2
Benzo[*b*]fluoranthene	6.08	5.96	6.12	2.0	0.7
Benzo[*k*]fluoranthene	6.26	5.40	6.12	13.7	2.2
Benzo[*ghi*]perylene	6.81	6.70	6.58	1.6	3.4
Benzo[*a*]pyrene	6.18	6.11	6.12	1.1	1.0
Carbon disulphide	2.00	1.94	1.94	3.0	3.0
Chlorobenzene	2.84	2.64	2.86	7.0	0.7
Chloroethene	1.38	1.62	1.52	17.4	10.1
2-Chlorophenol	2.15	2.16	2.15	0.5	0.0
α-Chlorotoluene	2.30	2.79	2.70	21.3	17.4
2-Chlorotoluene	3.42	3.18	3.35	7.0	2.0
Chrysene	5.73	5.52	5.66	3.7	1.2
p,p'-DDT	6.11	6.79	6.76	11.1	10.6
Dibenz[*ah*]anthracene	6.38	6.70	6.84	5.0	7.2
1,2-Dichlorobenzene	3.38	3.28	3.45	3.0	2.1
1,3-Dichlorobenzene	3.48	3.28	3.57	5.7	2.6
1,4-Dichlorobenzene	3.40	3.28	3.57	3.5	5.0
1,2-Dichloroethane	1.48	1.83	1.46	23.6	1.4
2,4-Dichlorophenol	3.23	2.80	2.97	13.3	8.0
Dichlorvos	1.34	0.60	1.79	55.2	33.6
Dieldrin	4.94	5.45	4.74	10.3	4.0
Endosulfan (α form)	3.69	3.50	4.47	5.1	21.1
Endosulfan (β form)	3.62	3.50	4.47	3.3	23.5
Ethylbenzene	3.15	3.03	3.17	3.8	0.6
Fenitrothion	3.44	3.30	3.21	4.1	6.7
Fluoranthene	5.13	4.22	4.95	17.7	3.5

Chemical	log K_{ow} (dimensionless)			Absolute error (per cent)	
	Literature	KOWWIN	CLOGP	KOWWIN	CLOGP
Hexachlorobenzene	5.47	5.86	6.06	7.1	10.8
Hexchloro-1,3-butadiene	4.86	4.72	4.90	2.9	0.8
α-Hexachlorocyclohexane	3.77	4.26	3.75	13.0	0.5
β-Hexachlorocyclohexane	3.87	4.26	3.75	10.1	3.1
γ-Hexachlorocyclohexane	3.67	4.26	3.75	16.1	2.2
Indeno[*123-cd*]pyrene	5.97	5.84	5.99	2.2	0.3
Malathion	2.90	2.29	2.48	21.0	14.5
Naphthalene	3.34	3.17	3.32	5.1	0.6
Pentachlorobenzene	5.03	5.22	5.35	3.8	6.4
Pentachlorophenol	5.07	4.74	4.71	6.5	7.1
Phenol	1.48	1.51	1.47	2.0	0.7
2-Propanone	-0.24	-0.24	-0.21	0.0	12.5
Pyrene	5.08	4.93	4.95	3.0	2.6
1,2,3,4-Tetrachlorobenzene	4.54	4.57	4.63	0.7	2.0
1,2,3,5-Tetrachlorobenzene	4.58	4.57	4.75	0.2	3.7
1,2,4,5-Tetrachlorobenzene	4.51	4.57	4.75	1.3	5.3
1,1,1,2-Tetrachloroethane	3.03	2.93	3.03	3.3	0.0
1,1,2,2-Tetrachloroethane	2.39	2.19	2.64	8.4	10.5
Tetrachloroethene	2.88	2.97	3.48	3.1	20.8
Tetrachloromethane	2.83	2.44	2.88	13.8	1.8
2,3,4,6-Tetrachlorophenol	4.42	4.09	4.00	7.5	9.5
Toluene	2.73	2.54	2.64	7.0	3.3
1,2,3-Trichlorobenzene	4.09	3.93	4.04	3.9	1.2
1,2,4-Trichlorobenzene	4.03	3.93	4.16	2.5	3.2
1,3,5-Trichlorobenzene	4.10	3.93	4.28	4.1	4.4
1,1,1-Trichloroethane	2.49	2.68	2.48	7.6	0.4
Trichloroethene	2.53	2.47	2.63	2.4	4.0
Trichloromethane	1.97	1.52	1.95	22.8	1.0
2,4,6-Trichlorophenol	3.69	3.45	3.39	6.5	8.1
α,α,α-Trichlorotoluene	2.92	3.90	4.12	33.6	41.1
Trifluralin	5.23	5.31	5.32	1.5	1.7
m-Xylene	3.20	3.09	3.14	3.4	1.9
o-Xylene	3.12	3.09	3.09	1.0	1.0
p-Xylene	3.15	3.09	3.14	1.9	0.3

			Average	7.8	5.8

Appendix I

Calculated values for the organic carbon-water partition coefficient (see 2.9.4 for further information)

Table I1: Comparison of measured and estimated values of the logarithm of the organic carbon-water partition coefficient (cm^3 g^{-1})

Chemical	log K_{oc} – linear regression models by chemical class (cm^3 g^{-1})						
	Predominantly hydrophobic	Non-hydrophobics	Phenols, anilines, benzo-nitriles, nitrobenzenes	Pesticides	Phenols, benzo-nitriles	Phosphates	Triazines
Aldrin	5.34						
Atrazine		2.45		2.38			2.33
Azinphos-methyl		2.42		2.35		2.49	2.31
Benzene	1.83						
Benzo[*a*]anthracene	4.89						
Benzo[*b*]fluoranthene	5.02						
Benzo[*k*]fluoranthene	5.17						
Benzo[*ghi*]perylene	5.62						
Benzo[*a*]pyrene	5.11						
Carbon disulphide		2.06					
Chlorobenzene	2.40						
Chloroethene	1.22						
2-Chlorophenol		2.14	2.25		2.31		
α-Chlorotoluene	1.96						
2-Chlorotoluene	2.87						
Chrysene	4.74						
p,p'-DDT	5.05						
Dibenz[*ah*]anthracene	5.27						
1,2-Dichlorobenzene	2.84						
1,3-Dichlorobenzene	2.92						
1,4-Dichlorobenzene	2.85						
1,2-Dichloroethane	1.30						
2,4-Dichlorophenol		2.70	2.93		2.92		
Dichlorvos		1.72		1.72		1.83	
Dieldrin		3.59					
Endosulfan (α form)		2.94					
Endosulfan (β form)		2.90					

Chemical	log K_{oc} – linear regression models by chemical class ($cm^3 g^{-1}$)						
	Predominantly hydrophobic	Non-hydrophobics	Phenols, anilines, benzo-nitriles, nitrobenzenes	Pesticides	Phenols, benzo-nitriles	Phosphates	Triazines
Ethylbenzene	2.65						
Fenitrothion		2.81		2.71		2.86	
Fluoranthene	4.26						
Hexachlorobenzene	4.53						
Hexchloro-1,3-butadiene	4.04						
α-Hexachlorocyclohexane	3.15						
β-Hexachlorocyclohexane	3.23						
γ-Hexachlorocyclohexane	3.07						
Indeno[*123-cd*]pyrene	4.94						
Malathion		2.53		2.45		2.59	
Naphthalene	2.81						
Pentachlorobenzene	4.17						
Pentachlorophenol		3.66	4.09		3.97		
Phenol		1.79	1.83		1.92		
2-Propanone		0.90					
Pyrene	4.21						
1,2,3,4-Tetrachlorobenzene	3.78						
1,2,3,5-Tetrachlorobenzene	3.81						
1,2,4,5-Tetrachlorobenzene	3.75						
1,1,1,2-Tetrachloroethane	2.55						
1,1,2,2-Tetrachloroethane	2.04						
Tetrachloroethene	2.43						
Tetrachloromethane	2.39						
2,3,4,6-Tetrachlorophenol		3.32	3.68		3.60		
Tetra ethyl lead[b]		3.56					
Toluene	2.31						
Tributyl tin oxide (TBTO)[b]		3.13					
1,2,3-Trichlorobenzene	3.41						
1,2,4-Trichlorobenzene	3.36						
1,3,5-Trichlorobenzene	3.42						
1,1,1-Trichloroethane	2.12						
Trichloroethene	2.15						
Trichloromethane	1.70						
2,4,6-Trichlorophenol		2.94	3.22		3.18		
α,α,α-Trichlorotoluene	2.47						

Chemical	log K_{oc} – linear regression models by chemical class ($cm^3 g^{-1}$)						
	Predominantly hydrophobic	**Non-hydrophobics**	**Phenols, anilines, benzo-nitriles, nitrobenzenes**	**Pesticides**	**Phenols, benzo-nitriles**	**Phosphates**	**Triazines**
Trifluralin		3.74	4.19				
m-Xylene	2.69						
o-Xylene	2.63						
p-Xylene	2.65						

Notes

[a] See Table A7 in Appendix A for the recommended literature value for log K_{ow}

[b] See Table H1 in Appendix H for the estimated log K_{ow} value for this chemical

Appendix J

Comparison of calculated values for the vapour pressure at 20 or 25°C with literature data and the recommended values at 10°C for use in the derivation of Soil Guideline Values (see 2.9.4 for further information)

Table J1: Comparison of experimental vapour pressure measurements (Pa) at 20 or 25°C and estimation methods

Chemical	Vapour pressure at 20 or 25°C (Pa)			Absolute error (per cent or order of magnitude)	
	Literature [a]	Grain-Watson	Modified Watson	Grain-Watson	Modified Watson
Aldrin	5.00E-03	8.03E-02	9.27E-04	one order	one order
Atrazine	4.00E-05	3.15E-03	1.00E-04	two orders	one order
Azinphos-methyl	3.00E-05	5.85E-08	8.01E-14	three orders	nine orders
Benzene	1.27E+04	1.30E+04	1.23E+04	2.7	3.2
Benzo[*a*]anthracene	2.80E-05	1.56E-05	8.31E-09	44.2	four orders
Benzo[*b*]fluoranthene	6.67E-05	4.05E-07	2.00E-11	two orders	six orders
Benzo[*k*]fluoranthene	1.28E-08	2.72E-07	7.96E-11	one order	three orders
Benzo[*ghi*]perylene	1.43E-08	3.44E-09	4.21E-13	one order	five orders
Benzo[*a*]pyrene	3.05E-06	3.25E-07	1.77E-11	one order	five orders
Carbon disulphide	4.80E+04	4.88E+04	4.76E+04	1.7	0.7
Chlorobenzene	1.58E+03	1.64E+03	1.53E+03	3.9	3.4
Chloroethene	3.55E+05	3.25E+05	3.22E+05	8.5	9.4
2-Chlorophenol	2.39E+02	2.27E+02	2.18E+02	5.1	9.0
α-Chlorotoluene	1.73E+02	1.96E+02	1.89E+02	13.5	9.4
2-Chlorotoluene	4.78E+02	5.31E+02	5.02E+02	11.1	5.0
Chrysene	6.93E-07	7.03E-07	3.20E-09	1.5	two orders
p,*p*'-DDT	2.00E-05	3.96E-01	1.36E-01	four orders	four orders
Dibenz[*ah*]anthracene	3.71E-10	3.69E-09	4.18E-13	one order	three orders
1,2-Dichlorobenzene	1.96E+02	2.04E+02	1.97E+02	4.1	0.6
1,3-Dichlorobenzene	2.81E+02	2.98E+02	2.86E+02	6.1	1.7
1,4-Dichlorobenzene	7.07E+01	1.56E+02	1.74E+02	one order	one order
1,2-Dichloroethane	1.05E+04	1.06E+04	9.97E+03	1.3	5.0
2,4-Dichlorophenol	1.19E+01	9.80E+01	8.77E+01	same order	same order
Dichlorvos	7.03E+00	1.06E+01	1.13E+01	51.1	60.9
Dieldrin	5.00E-04	7.11E-07	1.28E-10	three orders	six orders
Ethylbenzene	1.27E+03	1.36E+03	1.27E+03	7.5	0.1
Fluoranthene	3.13E-03	1.22E-03	2.11E-06	61.0	three orders
Hexachlorobenzene	1.45E-03	4.14E-04	1.24E-04	one order	one order

Chemical	Vapour pressure at 20 or 25°C (Pa)			Absolute error (per cent or order of magnitude)	
	Literature [a]	Grain-Watson	Modified Watson	Grain-Watson	Modified Watson
Hexchloro-1,3-butadiene	2.00E+01	9.31E+01	9.48E+01	same order	same order
α-Hexachlorocyclohexane	2.31E-01	4.77E-02	3.86E-02	one order	one order
β-Hexachlorocyclohexane	6.21E-05	1.76E-04	6.32E-04	two orders	one order
γ-Hexachlorocyclohexane	1.25E-03	1.47E-02	2.40E-04	one order	one order
Indeno[*123-cd*]pyrene	1.35E-08	3.95E-08	1.34E-13	same order	five orders
Malathion	1.00E-03	5.52E-03	9.84E-03	same order	same order
Naphthalene	1.04E+01	1.14E+01	2.01E+01	9.2	93.3
Pentachlorobenzene	2.20E-01	4.02E-01	6.36E-02	82.9	71.1
Pentachlorophenol	3.50E-02	2.37E-03	1.20E-03	one order	one order
Phenol	5.59E+01	5.46E+01	4.20E+01	2.3	24.9
2-Propanone	3.08E+04	3.20E+04	3.08E+04	3.9	0.1
Pyrene	1.65E-03	1.63E-04	3.47E-07	one order	four orders
1,2,3,4-Tetrachlorobenzene	3.03E+00	3.23E+00	3.37E-01	6.6	88.9
1,2,3,5-Tetrachlorobenzene	8.64E+00	4.03E+00	5.66E-01	53.4	93.4
1,2,4,5-Tetrachlorobenzene	6.67E-01	5.66E-01	6.24E-01	15.2	6.5
1,1,1,2-Tetrachloroethane	1.58E+03	1.80E+03	1.68E+03	14.1	6.2
1,1,2,2-Tetrachloroethane	7.93E+02	7.64E+02	7.14E+02	3.6	10.0
Tetrachloroethene	2.47E+03	2.41E+03	2.23E+03	2.5	9.5
Tetrachloromethane	1.53E+04	1.54E+04	1.45E+04	0.5	5.1
2,3,4,6-Tetrachlorophenol	2.80E-01	1.25E+00	1.77E-01	one order	36.8
Toluene	3.79E+03	3.95E+03	3.67E+03	4.2	3.2
1,2,3-Trichlorobenzene	7.23E+01	1.69E+01	1.52E+01	76.7	79.0
1,2,4-Trichlorobenzene	4.00E+01	4.13E+01	4.20E+01	3.2	5.0
1,3,5-Trichlorobenzene	7.73E+01	2.11E+01	2.54E+01	72.7	67.1
1,1,1-Trichloroethane	1.65E+04	1.68E+04	1.59E+04	1.9	3.5
Trichloroethene	9.77E+03	9.80E+03	9.18E+03	0.3	6.0
Trichloromethane	2.43E+04	2.68E+04	2.57E+04	10.2	5.6
2,4,6-Trichlorophenol	2.79E+00	1.09E+00	1.63E-01	60.8	94.2
α,α,α-Trichlorotoluene	4.60E+01	3.51E+01	3.63E+01	23.6	21.2
Trifluralin	1.50E-02	5.00E-04	9.44E-08	two orders	six orders
m-Xylene	1.11E+03	1.23E+03	1.15E+03	10.6	3.2
o-Xylene	1.17E+03	9.77E+02	9.14E+02	16.5	21.9
p-Xylene	1.17E+03	1.26E+03	1.18E+03	8.0	0.8

Notes

[a] See Table A8 in Appendix A

Table J2: Vapour pressures of liquids and solids at 10°C (Pa)

Chemical	Physical state at 10°C [a]	Vapour pressure at 10°C (Pa) [b]	
		Liquid or super-cooled liquid	Solid
Aldrin	solid	1.29E-01	1.35E-02
Atrazine	solid	2.43E-02	3.93E-04
Azinphos-methyl	solid	1.03E-08	2.37E-09
Benzene	liquid	6.24E+03	
Benzo[*a*]anthracene	solid	5.50E-05	1.24E-06
Benzo[*b*]fluoranthene	solid	3.46E-06	6.34E-08
Benzo[*k*]fluoranthene	solid	3.67E-06	1.64E-08
Benzo[*ghi*]perylene	solid	1.83E-07	1.55E-10
Benzo[*a*]pyrene	solid	1.58E-06	2.00E-08
Carbon disulphide	liquid	2.65E+04	
Chlorobenzene	liquid	6.73E+02	
Chloroethene	liquid	2.20E+05	
2-Chlorophenol	liquid	7.96E+01	
α-Chlorotoluene	liquid	6.85E+01	
2-Chlorotoluene	liquid	2.01E+02	
Chrysene	solid	3.19E-05	4.52E-08
p,p'-DDT	solid	6.53E-01	6.06E-02
Dibenz[*ah*]anthracene	solid	1.80E-07	1.66E-10
1,2-Dichlorobenzene	liquid	7.21E+01	
1,3-Dichlorobenzene	liquid	1.09E+02	
1,4-Dichlorobenzene	solid	1.02E+02	3.85E+01
1,2-Dichloroethane	liquid	4.92E+03	
2,4-Dichlorophenol	solid	5.59E+01	2.54E+01
Dichlorvos	liquid	2.95E+00	
Dieldrin	solid	2.82E-06	4.18E-08
Ethylbenzene	liquid	5.53E+02	
Fluoranthene	solid	1.48E-03	1.31E-04
Hexachlorobenzene	solid	2.76E-02	8.69E-05
Hexchloro-1,3-butadiene	liquid	3.30E+01	
α-Hexachlorocyclohexane	solid	2.67E-01	6.47E-03
β-Hexachlorocyclohexane	solid	7.48E-02	1.80E-05
γ-Hexachlorocyclohexane	solid	4.43E-02	3.70E-03
Indeno[*123-cd*]pyrene	solid	9.77E-08	2.12E-09
Malathion	liquid	9.22E-04	
Naphthalene	solid	1.20E+01	2.31E+00
Pentachlorobenzene	solid	3.81E-01	6.33E-02

Chemical	**Physical state at 10°C** [a]	**Vapour pressure at 10°C (Pa)** [b]	
		Liquid or super-cooled liquid	**Solid**
Pentachlorophenol	solid	1.57E-02	2.43E-04
Phenol	solid	2.29E+01	1.15E+01
2-Propanone	liquid	1.63E+04	
Pyrene	solid	5.13E-04	1.53E-05
1,2,3,4-Tetrachlorobenzene	solid	1.39E+00	5.97E-01
1,2,3,5-Tetrachlorobenzene	solid	2.08E+00	7.53E-01
1,2,4,5-Tetrachlorobenzene	solid	2.24E+00	9.04E-02
1,1,1,2-Tetrachloroethane	liquid	7.48E+02	
1,1,2,2-Tetrachloroethane	liquid	2.91E+02	
Tetrachloroethene	liquid	1.01E+03	
Tetrachloromethane	liquid	7.53E+03	
2,3,4,6-Tetrachlorophenol	solid	8.81E-01	2.19E-01
Tetraethyl lead	liquid	1.45E+00	
Toluene	liquid	1.73E+03	
Tributyl tin oxide	liquid	8.56E-04	
1,2,3-Trichlorobenzene	solid	8.93E+00	3.50E+00
1,2,4-Trichlorobenzene	solid	1.29E+01	1.11E+01
1,3,5-Trichlorobenzene	solid	1.49E+01	4.41E+00
1,1,1-Trichloroethane	liquid	8.25E+03	
Trichloroethene	liquid	4.58E+03	
Trichloromethane	liquid	1.35E+04	
2,4,6-Trichlorophenol	solid	6.83E-01	1.74E-01
α,α,α-Trichlorotoluene	liquid	1.10E+01	
Trifluralin	solid	1.08E-04	4.46E-05
m-Xylene	liquid	4.95E+02	
o-Xylene	liquid	3.86E+02	
p-Xylene	solid	5.10E+02	4.75E+02

Notes

[a] Estimated from boiling point and melting point

[b] Estimated using the Grain-Watson method (Boethling and Mackay 2000)

Appendix K

Comparison of water solubility data from the literature at 10 and 25°C, along with different estimation methods for water solubility at 25°C (see 2.10.4 for further information)

Table K1: Comparison of experimental data for water solubility (mg L^{-1}) at 10 and 25°C from the IUPAC-NIST Solubility Database

Chemical	**Water solubility (mg L^{-1})**		**Absolute difference (per cent)**
	10°C	**25°C**	
Benzene	1.78E+03	1.77E+03	0.6
Chlorobenzene	4.54E+02	4.93E+02	8.6
1,2-Dichlorobenzene	1.33E+02	1.46E+02	9.8
1,3-Dichlorobenzene	1.03E+02	1.06E+02	2.9
1,4-Dichlorobenzene	5.12E+01	8.26E+01	61.3
1,2-Dichloroethane	8.68E+03	8.60E+03	0.9
Ethylbenzene	1.80E+02	1.69E+02	6.1
Naphthalene	1.90E+01	3.10E+01	63.2
1,1,1,2-Tetrachloroethane	1.11E+03	1.07E+03	3.6
1,1,2,2-Tetrachloroethane	2.93E+03	2.83E+03	3.4
Tetrachloroethene	2.25E+02	2.06E+02	8.4
Tetrachloromethane	8.46E+02	8.13E+02	3.9
Toluene	5.90E+02	5.30E+02	10.2
1,1,1-Trichloroethane	1.30E+03	1.29E+03	0.8
Trichloroethene	1.37E+03	1.28E+03	6.6
Trichloromethane	8.95E+03	7.98E+03	10.8
m-Xylene	2.00E+02	1.60E+02	20.0
p-Xylene	2.00E+02	1.80E+02	10.0
		Average	12.8

Table K2: Comparison of recommended literature values and estimated values for water solubility (mg L^{-1}) at 25°C

Chemical	Water solubility at 25°C (mg L^{-1})				Absolute error (per cent or order of magnitude)		
	Literature [a]	K_{ow} method	WSKOWIN method	AQUAFAC method	K_{ow} method	WSKOWIN method	AQUAFAC method
Aldrin	2.00E-02	6.06E-03	1.48E-02	6.40E-02	69.7	25.8	same order
Atrazine	7.00E+01	3.31E+01	2.25E+01	1.08E+02	52.8	67.9	one order
Benzene	1.77E+03	2.14E+03	1.98E+03	9.26E+02	20.8	11.6	47.7
Benzo[*a*]anthracene	1.10E-02	5.18E-03	2.59E-02	1.72E-02	52.9	same order	56.3
Benzo[*k*]fluoranthene	8.00E-04	5.69E-04	3.33E-03	1.19E-03	28.9	one order	48.9
Benzo[*ghi*]perylene	2.60E-04	3.56E-05	2.83E-04	8.36E-05	one order	8.8	67.8
Benzo[*a*]pyrene	3.80E-03	1.64E-03	8.57E-03	2.72E-03	56.9	same order	28.4
Chlorobenzene	4.84E+02	3.99E+02	4.62E+02	3.25E+02	17.5	4.6	32.8
Chloroethene	2.76E+03	1.48E+04	9.29E+03	1.56E+03	one order	same order	43.6
2-Chlorophenol	2.27E+04	3.32E+03	1.97E+04	1.50E+04	85.4	13.1	33.9
2-Chlorotoluene	1.17E+02	8.46E+01	1.30E+02	1.43E+02	27.7	11.2	22.2
Chrysene	2.00E-03	9.75E-04	5.16E-03	1.93E-03	51.3	same order	3.5
p,*p*'-DDT	5.70E-03	1.50E-02	3.12E-02	1.47E-02	one order	one order	one order
Dibenz[*ah*]anthracene	6.00E-04	1.33E-04	7.74E-04	8.95E-05	77.9	29.0	85.1
1,2-Dichlorobenzene	1.45E+02	1.10E+02	1.43E+02	1.04E+02	24.0	1.6	28.6
1,3-Dichlorobenzene	1.06E+02	8.27E+01	1.14E+02	1.04E+02	22.0	7.9	2.3
1,4-Dichlorobenzene	8.26E+01	5.44E+01	7.52E+01	5.41E+01	34.2	8.9	34.5
1,2-Dichloroethane	8.60E+03	1.76E+04	9.05E+03	1.34E+03	one order	5.2	84.4
2,4-Dichlorophenol	4.50E+03	1.18E+02	1.17E+03	2.91E+03	one order	74.0	35.3
Dieldrin	2.00E-01	9.97E-02	8.91E-02	1.91E+00	50.1	55.5	one order
Endosulfan (α form)	5.30E-01	1.93E+01	5.45E+00		two orders	one order	
Endosulfan (β form)	2.80E-01	2.25E+00	7.34E-01		one order	same order	
Ethylbenzene	1.61E+02	1.54E+02	2.30E+02	1.45E+02	4.1	42.9	10.2
Fluoranthene	2.30E-01	1.38E-01	4.49E-01	2.13E-01	39.9	same order	7.3
Hexachlorobenzene	9.60E-03	4.75E-03	1.34E-02	6.46E-03	50.5	39.4	32.7
Hexchloro-1,3-butadiene	4.80E+00	2.76E+00	4.22E+00	5.63E+00	42.5	12.1	17.2
α-Hexachlorocyclohexane	2.00E+00	3.30E+00	2.51E+00	2.22E+00	65.2	25.5	10.8
β-Hexachlorocyclohexane	2.00E-01	6.97E-02	7.53E-02	6.23E-02	65.2	62.4	68.8
γ-Hexachlorocyclohexane	7.30E+00	1.26E+01	8.22E+00	6.32E+00	72.1	12.5	13.4
Malathion	1.45E+02	9.86E+02	2.46E+02		same order	69.7	
Naphthalene	3.10E+01	3.01E+01	4.82E+01	2.23E+01	2.9	55.4	28.2
Pentachlorobenzene	5.00E-01	3.97E-01	8.21E-01	6.24E-01	20.6	64.3	24.9
Phenol	8.41E+04	1.16E+04	5.82E+04	3.12E+04	86.2	30.8	62.9

Chemical	**Water solubility at 25°C (mg L^{-1})**				**Absolute error (per cent or order of magnitude)**		
	Literature [a]	**K_{ow} method**	**WSKOWIN method**	**AQUAFAC method**	**K_{ow} method**	**WSKOWIN method**	**AQUAFAC method**
2-Propanone	4.41E+05	1.46E+06	3.20E+05	2.09E+04	one order	27.5	one order
Pyrene	1.30E-01	6.28E-02	2.14E-01	8.39E-02	51.7	64.8	35.4
1,2,3,4-Tetrachlorobenzene	7.80E+00	3.41E+00	6.07E+00	5.36E+00	56.3	22.2	31.3
1,2,3,5-Tetrachlorobenzene	3.50E+00	2.58E+00	4.79E+00	4.56E+00	26.2	36.8	30.4
1,2,4,5-Tetrachlorobenzene	6.00E-01	4.46E-01	9.23E-01	6.45E-01	25.6	53.8	7.4
1,1,1,2-Tetrachloroethane	1.07E+03	3.45E+02	3.03E+02	1.27E+03	67.8	same order	19.0
1,1,2,2-Tetrachloroethane	2.83E+03	2.17E+03	1.25E+03	1.15E+03	23.2	55.8	59.5
Tetrachloroethene	1.50E+02	5.24E+02	4.23E+02	3.15E+02	same order	same order	same order
Tetrachloromethane	8.00E+02	5.62E+02	4.79E+02	4.09E+03	29.8	40.2	one order
2,3,4,6-Tetrachlorophenol	1.83E+02	3.08E+00	4.30E+01	1.38E+02	two orders	76.5	24.3
Toluene	5.22E+02	4.49E+02	5.59E+02	4.27E+02	14.0	7.1	18.2
1,2,3-Trichlorobenzene	2.10E+01	9.58E+00	1.63E+01	1.69E+01	54.4	22.3	19.4
1,2,4-Trichlorobenzene	4.14E+01	2.10E+01	3.26E+01	3.12E+01	49.4	21.3	24.7
1,3,5-Trichlorobenzene	6.00E+00	7.14E+00	2.79E+01	1.30E+01	19.0	one order	one order
1,1,1-Trichloroethane	1.29E+03	1.30E+03	1.02E+03	1.71E+03	0.5	20.8	32.6
Trichloroethene	1.10E+03	1.14E+03	9.34E+02	5.40E+02	3.4	15.0	50.9
Trichloromethane	7.98E+03	5.18E+03	3.19E+03	4.03E+03	35.1	60.0	49.5
2,4,6-Trichlorophenol	4.34E+02	2.19E+01	2.41E+02	4.95E+02	one order	44.5	14.0
Trifluralin	1.00E+00	7.01E-01	8.38E-01	9.15E-03	29.9	16.2	two orders
m-Xylene	1.61E+02	1.34E+02	2.06E+02	1.92E+02	17.0	28.0	19.4
o-Xylene	1.73E+02	1.68E+02	2.45E+02	1.92E+02	2.7	41.9	11.2
p-Xylene	1.81E+02	1.54E+02	2.30E+02	1.92E+02	14.7	27.2	6.2

Notes

[a] See Table A9 in Appendix A

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