1 of 3

Intermedia Transfer Factors for Fifteen Toxic Pollutants Released to Air Basins in California

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FORWARD AND ACKNOWLEDGEMENTS

As part of an effort to improve the Health Risk Assessment (HRA) computer program developed by the State of California Air Resources Board (ARB), the scientific objectives of this project are to develop for toxic chemical emissions to air the intermedia transfer factors (ITFs) to be used for estimating contaminant partitioning between air, soil, water, sediments, and biota. These ITFs will be compatible with both current and improved versions of the HRA model as well as other models that require ITF inputs.

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INTRODUCTION

The purpose of this report is to provide intermedia-transfer factors (ITFs) for 15 chemicals. For these chemicals we have carried out a critical review of the existing literature in order to identify a range and best estimate values for the following ITFs:

- molecular weight
- melting point
- octanol-water partition coefficient (K_{ow})
- vapor pressure at standard temperature (VP)
- solubility in water (WS)
- Henry's law constant (H)
- organic-carbon partition coefficient (K_{oc})
- soil-water and/or sediment-water partition coefficient (K_d)
- diffusion coefficient in water (D_{water})
- diffusion coefficient in air (D_{air})
- Bioconcentration factors for plant tissue concentration relative to soil concentration (K_{ps})
- Bioconcentration factors for plant leaf concentration relative to air concentration (K_{pa})
- Bioconcentration factors for fish-tissue concentration relative to water/or sediment concentrations (BCF)
- Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle (B_k)
- Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens (B_l)
- Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens (B_e)
- Contaminant biodegradation factors in soil
- Media-specific half lives for air, soil, and surface water

For factors that are not directly available from the literature, including references such as Lyman *et al.* (1990), Verschueren (1983), Howard (1989), Howard *et al.* (1990, 1991) and Mackay *et al.* (1992a, 1992b, 1993); we discuss here methods to calculate these factors.

This report is divided into two parts, in the first part we provide a summary definition of the ITFs, discuss methods for estimating these parameters in the absence of measured values, and consider the estimation errors inherent in these estimation methods. In the second part, we provide a detailed summaries of measured and estimated ITF values for 15 air contaminants and make recommendations regarding the expected value and variance in these values for use in exposure models.

PART I: SUMMARY DEFINITION OF ITFs

DEFINITIONS OF INTERMEDIA TRANSFER FACTORS

The use of any multimedia transport model relating contaminant concentrations in air to those in soil, water, and biota, requires that we determine the intermedia transfer factors (ITFs) that define concentration relationships between an exposure medium and the environmental medium that provides contaminant to the exposure medium. In this section, we consider how ITFs are used in a generalized exposure model and we define the ITFs for which values are presented in Part II of this report.

The Basic Exposure Model and ITFs

The exposure-assessment process relates contaminant concentrations in environmental media—air, surface soil, root-zone soil, surface water, and ground water, etc.—to contaminant concentrations in the exposure media with which a human population has contact (personal air, tap water, foods, household dusts and soils, etc.). Average daily dose within an exposed population is the product of the exposure concentrations in these contact media and an intake or uptake factor that relates the concentrations to the distributions of potential dose by the inhalation, ingestion, and dermal contact routes within the population. Thus, the population-averaged potential dose during a period of time when environmental concentrations remain constant is expressed as an average daily dose rate (ADD), in mg/kg-d,

$$ADD = \left[\frac{C_i}{C_k} \right] \times \left[\frac{IU_i}{BW} \right] \times \frac{EF \times ED}{AT} \times C_k \quad , \quad [1]$$

where $[C_i/C_k]$ is the intermedia concentration ratio, which expresses the ratio of contaminant concentration in the *exposure* medium i to the concentration in an environmental medium k ; $[IU_i/BW]$ is the intake or uptake factor per unit body weight associated with the exposure medium i ; EF is the exposure frequency for the exposed population, in days per year; ED is the exposure duration for the exposed population, in years; AT is the averaging time for the exposed population, in days; and C_k is the contaminant concentration in environmental medium k . For exposure through the ingestion route, $[IU_i/BW]$ is the intake rate per unit body weight of the exposure medium such as kg(vegetables)/kg-d, L(milk)/kg-d, or kg(meat)/kg-d. The calculation of the intermedia concentration ratio, C_i/C_k , requires the use of the ITFs described in the sections below. The reliability of the intermedia concentration ratio is directly dependent on the reliability in the measured and estimated values of the ITFs which are used to calculate this ratio.

Molecular Weight

Molecular weight is the mass of one gram-mole of an element or compound, that is the mass of 6.02252×10^{23} atoms or molecules.

Melting Point

The melting point is the temperature at which a compound makes the transition from a solid to a liquid phase. It is typically measured at atmospheric pressure.

Octanol-Water Partition Coefficient, K_{ow}

The octanol-water partition coefficient provides a measure of the extent of chemical partitioning between water and octanol at equilibrium. The greater the K_{ow} , the more likely a chemical is to partition to octanol than to water. The octanol-water partition coefficient is used as a basis for estimating organic carbon partitioning in soils and sediments, bioconcentration factors in aquatic organisms, root-soil and leaf-air partition coefficients in land vegetation, and fat-diet partition coefficients in terrestrial animals.

Vapor Pressure, VP

Vapor pressure is a saturation property in that it is a measure of the maximum capacity that a gas phase medium has for a chemical. VP is the pressure exerted by a chemical vapor in equilibrium with its solid or liquid phase. It is used to calculate the rate of volatilization of contaminant from soil or water and for estimating the Henry's law constant for low-solubility chemicals. The higher the vapor pressure, the more likely a chemical is to exist in the gas phase.

Water Solubility, WS

Water solubility is also a saturation property in that it is a measure of the capacity of the water phase to hold a contaminant. WS is the upper limit on a chemical's dissolved concentration in pure water at a specified temperature.

Henry's Law Constant, H

This factor is a measure at equilibrium of the ratio of chemical activity in the gas above a liquid to chemical activity in the liquid. It is the basis for estimating air-water partition coefficients and is often expressed as the partial pressure of chemical in the gas phase divided by the concentration in the water phase. For chemicals with a low solubility limit in water, the Henry's law constant can be estimated as the vapor pressure of the pure chemical divided by the solubility limit in water. The higher the Henry's law constant, the more likely a chemical is to exist in the gaseous state than remain dissolved in water.

Organic-Carbon Partition Coefficient, K_{oc}

The organic-carbon partition coefficient provides a measure of chemical partitioning between organic carbon (in soils and sediments) and water. The higher the K_{oc} , the more likely a chemical is to bind to the solid phase of soil or sediment than to the liquid phase. When K_{oc} is multiplied by the fraction organic carbon in a soil or sediment, we obtain an estimate of the soil/water or sediment/water partition coefficient.

The Soil-Water Distribution Coefficient, K_d

K_d represents the distribution or sorption coefficient, which is the ratio at equilibrium of chemical concentration attached to particles (mol/kg) to chemical concentration in the solution, mol/L.

Diffusion Coefficients in Air and Water

Diffusion coefficients describe the movement of a molecule in a liquid or gas medium as a result of differences in concentration. They are used to calculate the dispersive component of chemical transport. The higher the diffusion coefficient, the more likely a chemical is to move in response to concentration gradients. Diffusive mass transfer at compartment boundaries is often modeled using a boundary layer model. The flux of contaminant from the surface to the bulk fluid is proportional to the difference in concentration between the surface and the bulk fluid. This approach is used for mass transfer between air and soil, air and surface water, and surface water and sediments. In order to carry out this approach, one needs estimates of the diffusion coefficients of a chemical in both pure air and pure water.

Bioconcentration Factors (BCFs)

Bioconcentration factors provide a measure of chemical partitioning between a biological medium such as fish tissue or plant tissue and an external medium such as water (for fish) or air (for plants). The higher the BCF the more likely partitioning in biota is likely to be high. BCFs have been expressed for fish/sediment, fish/water, plant-leaf/air, plant-root/soil, and animal-fat/diet partitioning.

Biotransfer Factors

Biotransfer factors are the steady-state contaminant concentration in fresh meat, milk, dairy products and eggs divided by the animals' daily contaminant intake and have units of $(\text{mg/kg})/(\text{mg/d})$ or d/kg . Unlike bioconcentration factors, which express steady-state concentration ratios between animal tissue and a specific environmental medium, biotransfer factors express the steady-state relationship between intake and tissue or food-product concentrations. For terrestrial animals that are exposed to contaminants from multiple media (such as air, water, forage, soil, etc.), the biotransfer factor has more utility for assessing the effects of multimedia contamination on food contamination.

Biodegradation Factors

The transformation of organic and inorganic compounds by microorganisms that are present in environmental media can have a profound influence on their

persistence and toxicity. Due to their broad range of enzymatic capabilities, microorganisms are capable of transforming many inorganic and organic compounds. Such transformations can result in the partial degradation of a compound (e.g., conversion of DDT to DDE), mineralization (i.e., complete transformation to carbon dioxide and water), or synthesis of a stable product (e.g., formation of methyl arsenicals from arsenate). While these processes generally result in the detoxification of the parent compound, other toxic products may also be formed. For example, the microbial metabolism of aromatic amines can result in the formation of mutagenic byproducts.

Media-Specific Half Lives

A medium-specific half life provides a relative measure of the persistence of a chemical in a given medium such as soil or water. This measure accounts for the sum of all loss mechanisms, both transport and transformation. The greater the half-life in a medium, the more persistent a chemical is likely to be in that medium.

INTERMEDIA TRANSFER FACTORS:

MEASURED VALUES AND ESTIMATION METHODS

Estimation Errors

For all the ITFs presented here the value of the ITF is described both by an arithmetic mean value and a coefficient of variation, which is the arithmetic standard deviation divided by the arithmetic mean and abbreviated as CV. The CV is used to describe measurement variance for properties that are measured and estimation error for properties that are estimated.

Estimates of many ITF properties are often based on regression equations that relate these ITFs to some measure of structure or activity associated with the contaminant. These methods are referred to as quantitative structure-activity relationship (QSAR) methods. It should be recognized that the reliability of an exposure model will be limited by the precision of these QSAR estimates. When these chemical properties are then used to estimate ITFs, the associated estimation errors are often not reported (see for example Travis and Arms, 1988).

Our estimate of precision in ITFs is based on calculating, S_e , the *standard error of the estimate* (or standard deviation of the residuals) in the regression equations and fragment models used to derive an ITF. The S_e for an ITF, such as the organic-carbon partition coefficient (K_{oc}) derived from a regression or

correlation analysis can be estimated according to the following formula (Hamburg, 1970),

$$S_e \text{ of } \log K_{oc}^{est} = \sqrt{\frac{1}{(n-2)} \sum_{i=1}^n [\log K_{oc}^{msd} - \log K_{oc}^{est}]^2} \quad [2]$$

where n is the number of chemicals used in the estimation protocol and K_{oc}^{est} refers to the estimated property (K_{oc} in this case) and K_{oc}^{msd} refers to the corresponding measured values used to carry out the regression.

Molecular Weight

For most organic and inorganic compounds, the molecular weight can be reliably obtained from a number of common references. The precision with which molecular weights can be measured is as high as ITF.

Melting Point

The melting point is a measured parameter and available for most compounds in the literature. Methods for estimating the melting point in the absence of measured values are describe by Lyman et al. (1990).

Octanol-Water Partition Coefficient, K_{ow}

Measured values of K_{ow} are available for many compounds. Experimental methods for measuring K_{ow} involve the determination of chemical concentration in water and octanol phases. This process is typically carried out using shake-flask or generator-column methods. Details of experimental methods are described in several papers, most notably in Fujita et al. (1964), Leo et al. (1971), Chiou et al. (1982), and De Bruijn et al. (1989). Literature reviews of measured and calculated values of K_{ow} for many contaminants are available in Howard (1989), Howard et al. (1990), Mackay et al. (1992a, 1992b, 1993), and Verschueren (1983). Methods for estimating K_{ow} are summarized in Lyman et al. (1990) and Verschueren (1983).

Vapor Pressure at Standard Temperature, VP

Measured values for vapor pressure are widely available. One of the earliest and most extensive compilations of vapor pressure for both organic and inorganic chemicals are those of Stull (1947a, 1947b).

In principal the determination of vapor pressure involves the measurement of saturation concentration or pressure of the solute in a gas phase. The most reliable methods involve direct determination of these concentrations but convenient indirect methods are also available. based on an evaporation rate measurement or chromatographic retention times. Vapor pressures are strongly dependent on temperature. Vapor pressure data are often regressed against temperature using and Antoine equation.

Literature reviews of measured values of VP for many contaminants are available in Boublik et al. (1984), Howard (1989), Howard et al. (1990), Mackay et al. (1992a, 1992b, 1993), Stull (1947a, 1947b), and Verschueren (1983). Methods for measuring VP are summarized in Lyman et al. (1990) and Mackay et al. (1992a, 1992b, 1993).

Solubility in Water, WS

Measured values for the solubility limit in water are also widely available. For most organic chemicals, the solubility is reported at a defined temperature in distilled water. Literature reviews of measured values of WS for many contaminants are available in Horvath (1982), Howard (1989), Howard et al. (1990), Mackay et al. (1992a, 1992b, 1993), Stephen and Stephen (1963), and Verschueren (1983). Methods for estimating WS in the absence of measure values are described in Lyman et al. (1990). Methods for measuring WS are described in Lyman et al. (1990) and Mackay et al. (1992a, 1992b, 1993).

Henry's Law Constant

The Henry's law constant is essentially an air-water partition coefficient that can be determined by measurement of solute concentrations in both phases. Literature reviews of measured values of H for many contaminants are available in Mackay and Shiu (1981), Howard (1989), Howard et al. (1990), Mackay et al. (1992a, 1992b, 1993), and Verschueren (1983). Methods for estimating H in the absence of measure values are summarized in Lyman et al. (1990). Methods for measuring H are summarized and described in Lyman et al. (1990) and Mackay et al. (1992a, 1992b, 1993).

Organic-Carbon Partition Coefficient, K_{oc} , and Sorption Coefficients, K_d

The organic-carbon partition coefficient provides a measure of chemical partitioning between organic carbon (in soils and sediments) and water. The higher the K_{oc} , the more likely a chemical is to bind to the solid phase of soil or sediment than to the liquid phase.

As reported in Lyman et al. (1990), Kenaga and Goring (1980) developed a regression for K_{oc} based on K_{ow} for a wide variety of compounds including many pesticides. This regression takes the form,

$$\log K_{oc} = 0.544 \log K_{ow} + 1.377 \text{ (45 compounds, many pesticides).} \quad [3]$$

Karickhoff (1985) has described several empirical estimation methods for obtaining K_{oc} from K_{ow} .

$$\log K_{oc} = 0.72 \log K_{ow} + 0.49 \text{ (methylated and halogenated benzenes)} \quad [4]$$

$$\log K_{oc} = 1.029 \log K_{ow} - 0.18 \text{ (13 pesticides)} \quad [5]$$

$$\log K_{oc} = 0.989 \log K_{ow} - 0.346 \text{ (5 poly-nuclear aromatics [PNAs])} \quad [6]$$

$$\log K_{oc} = \log K_{ow} - 0.317 \text{ (22 PNAs and substituted PNAs)} \quad [7]$$

These estimation equations can estimate K_{oc} with a CV of about 1. This estimation error does not include uncertainty in the value of K_{ow} . These estimation methods are intended for nonionic organic compounds. A larger CV should be expected when the estimation is applied to ionic species and a correction for acid dissociation should be made.

Chiou et al. (1977) have related K_{oc} to water solubility, S' in $\mu\text{mol/L}$, as

$$\log K_{oc} = 4.277 - 0.557 \log S' \text{ (15 chlorinated hydrocarbons)} \quad [8]$$

Kenaga (1980b) has related K_{oc} to water solubility (WS) in ppm

$$\log K_{oc} = 3.64 - 0.55 \log WS \text{ (358 compounds, mostly pesticides).} \quad [9]$$

Meylan et al (1992) have related K_{oc} to the molecular connectivity index ($^1\chi$).

The Soil-Water Distribution Coefficient, K_d

K_d represents the distribution or sorption coefficient, which at equilibrium is the ratio of chemical concentration attached to soil or sediment particles (mol/kg) to chemical concentration in the solution, mol/L. When K_{oc} for an organic compound is multiplied by the fraction of organic carbon in a soil or sediment, we obtain an estimate of the soil/water or sediment/water partition coefficient, K_d (Karickhoff, 1985). The CV in this estimation is dominated by the estimation error in K_{oc} and equal to 1.0. For inorganic chemicals, values of K_d can be based on measured values or on estimation methods both of which are discussed in Bodek et al. (1988).

Molecular Diffusion Coefficients

Molecular diffusion is the net transport of a molecule in a liquid or gas phase and is the result of intermolecular collisions rather than turbulence or bulk transport. Mass transport via molecular diffusion is driven by concentration gradients. A diffusion coefficient depends on properties of both the chemical species being transported and the phase or phases through which it is transported.

Diffusion in Water

Reid et al. (1987) and Lyman et al. (1990) have also reviewed several methods for estimating liquid diffusion coefficients and found these methods are all based on the Stokes-Einstein equation relating diffusivity to the temperature and viscosity of the solvent and the molecular radius of the solute. As noted by Reid et al. (1987), one of the oldest but still widely used empirical estimation methods for binary diffusion in liquids is that of Wilke and Chang (1955),

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}}, \quad [10]$$

where D_{xy} is the diffusion coefficient in of solute x in solvent y , m^2/d ; ϕ is the association factor of solvent y , no units; M_y is the molecular weight of the solvent, g/mol; T is the temperature of the solute-solvent system, K; η_y is the viscosity of the

solvent η , cP; and V_x is molecular volume of the solute at its normal boiling temperature, cm^3/mol . Wilke and Chang (1955) report an average estimation error of 10 per cent in predicting diffusion coefficients for 251 solute-solvent systems. They recommend an association factor of 2.6 when the solvent is water. The viscosity of water is 0.79 cP at 30 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). For many organic compounds, D_{water} is in the range of 10^{-5} to $10^{-4} \text{ m}^2/\text{d}$.

Diffusion in Air

Analytical methods for estimating the diffusion coefficient of a binary gas system have been reviewed by Reid et al. (1987) and Lyman et al. (1990). These methods have their foundations in a theoretical relationship referred to as the Chapman-Enskog model for dilute gases at low pressures (Chapman and Cowling, 1939; Reid et al., 1987). Based on accuracy and ease of use, Lyman et al. (1990) recommend two methods for use under ambient environmental conditions. When applied at atmospheric pressure, the most straightforward of these two methods relates diffusion in air to the molecular weight of the compound as

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}, \quad [11]$$

where D_{air} is the diffusion coefficient in air for compound x in m^2/d , T is the air temperature in K, M_x is the molecular weight of compound x in g/mol, and V_x is the molecular volume of the compound x in cm^3/mol . The values 29 and 2.7 represent the molecular weight and cubic root of molecular volume, respectively, for air. Methods for estimating molecular volumes are reviewed in Lyman et al. (1990). For many organic compounds, D_{air} is in the range of 0.1 to $1 \text{ m}^2/\text{d}$.

Plant-Soil Partition Coefficients, $K_{\text{ps}}^{\text{rain}}$, K_{ps} , and $K_{\text{ps}}(\text{roots})$

The plant-soil partition coefficients express the ratio of contaminant concentration in plant parts, both pasture and food, in mg/kg(plant fresh mass) to concentration in dry soil in mg/kg. We consider separately plant-soil partition coefficients for *surface soil*, which is roughly the top 1 cm of soil and for which the

mechanisms of transport from soil to plant are particle resuspension by wind and by rainsplash, and for *root-zone soil*, which is the soil layer from the bottom of the surface soil layer to the depth to which food crops and pasture crops extend their roots and is equal to roughly 1 m.

The transfer from surface soil to plant surfaces by wind erosion and subsequent deposition of contaminants attached to soil particles in the air is covered by the combination of contaminant concentration in air and the partition factor K_{pa}^{pt} described above. Thus, the only factor we include in the partition factor from surface soil to edible plant parts is the rainsplash partition factor, K_{ps}^{rain} . Dreicer et al. (1984) have shown that the value of the ratio of contaminant concentration on plant surfaces in mg/kg(plant dry mass) to contaminant concentration in soil is 1.7×10^{-2} with a geometric standard deviation of approximately 2.5. We adjust this to a fresh mass ratio (assuming that the plant dry-mass fraction equals 0.2) to obtain K_{ps}^{rain} equal to 3.4×10^{-3} with a CV of 1. This partition factor applies to both organic and inorganic contaminants.

The partition coefficient K_{ps} expresses the ratio of contaminant concentration (mg/kg) in the fresh mass of the edible portion of vegetation and pasture to the contaminant concentration in the root zone. This partition coefficient actually involves two partition factors, one between roots and soil and a second between edible plant parts and roots. When consideration is given to root crops, the second of these is unity. What is meant by the "concentration in a plant" can be difficult to define in larger plants where roots, stems, and leaves each may have different chemical concentrations. Recent studies on the bioconcentration of nonionic organic chemicals has focused on correlations between partition factors and known chemical properties, such as Henry's law constants (H) and octanol-water partition coefficients (K_{ow}) (Bacci et al., 1990; Briggs et al., 1982; Briggs et al., 1983; Travis and Hattemer-Frey, 1988; Travis and Arms, 1988). Ryan et al. (1988) and Riederer (1990) report the potential unreliability of simple plant/soil partition coefficients. McFarlane et al. (1987) have demonstrated experimentally that chemicals with similar values of K_{ow} can have drastically different long-term partitioning, probably due to differences in metabolism. Nonetheless, the plant-soil partition coefficient provides a simple and useful method for assessing potential dose. We use it here, recognizing its potentially large uncertainties. Briggs et al. (1982, 1983) have developed an estimation equation for uptake of contaminants by roots from soil solution. They refer to this partition coefficient as the root concentration factor,

RCF. It represents the ratio of contaminant concentration in root, mg/kg(fresh mass), to contaminant concentration in soil solution, mg/L, and it takes the form

$$RCF = 0.82 + 0.03 K_{ow}^{0.77} . \quad [12]$$

When this factor is divided by the sorption coefficient, $K_D = f_{oc} \times K_{oc} = 0.02 \times 0.411 \times K_{ow}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg(fresh mass) to contaminant concentration in soil solids, mg/kg, which we refer to as $K_{ps}(\text{roots})$ and estimate as

$$K_{ps}(\text{roots}) = 100 K_{ow}^{-1} + 3.7 K_{ow}^{-0.23} . \quad [13]$$

Based on studies of carbon-14-labeled organic chemicals in barley and cress, Topp et al. (1986) developed a correlation for the root-soil partition coefficient in terms of K_{oc} ,

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} . \quad [14]$$

with our substitution of $K_{oc} = 0.411 K_{ow}$ from above gives

$$K_{ps}(\text{roots}) = 273 K_{ow}^{-0.622} . \quad [15]$$

Based on a review of reported measurements of bioconcentration for 29 persistent organochlorines in plants, Travis and Arms (1988) have correlated plant-soil bioconcentration (on a dry-mass basis) in above-ground plant parts with octanol-water partition coefficients. This bioconcentration factor, B_v , on a dry-weight basis is expressed as

$$\log B_v = 1.58 - 0.58 \log K_{ow} \pm 0.73 \quad (n=29, r^2=0.525) \quad [16]$$

We calculated the error term, ± 0.73 , from the mean square error of the estimator for this regression from the data provided by Travis and Arms (1988). The geometric standard deviation in this estimate of B_v is $10^{(0.73)} (=5.4)$. This estimation error corresponds to a CV of 4. When adjusted to a fresh-mass basis, equation [16] gives

the plant-soil partition coefficient, K_{ps} , expressing the ratio of contaminant concentration in mg/kg in above-ground plant fresh relative to contaminant concentration in mg/kg (dry soil) in the root-zone soil,

$$K_{ps} = 7.7 K_{ow}^{-0.58} . \quad [17]$$

We recommend equation [17] to estimate the partitioning of organic contaminants between root-zone soil and above ground plant parts in order to calculate contaminant exposures for exposed produce. Because the estimates of K_{ps} from equations [13] and [15] do not differ by more than a factor of 3 over $10^3 < K_{ow} < 10^6$, and because equation [15] differs from equation [17] almost exactly a factor of 35, we estimate the partitioning of organic contaminants between root-zone soil and roots as

$$K_{ps}(\text{roots}) = 35 K_{ps} = 270 K_{ow}^{-0.58} \quad [18]$$

and recommend this as a basis for estimating contaminant concentrations in the edible root crops and other protected produce.

Bodek et al. (1988) have reviewed estimation methods for obtaining plant-soil partition coefficients for inorganic chemicals. For some inorganic chemicals, the literature on radionuclides is often a useful source for plant-soil partition factors (for example, see Ng, 1982). Regional scale biogeochemical partitioning between soil and plants as described by Bowen (1979) is useful for making preliminary estimates of plant-soil partitioning for some inorganic contaminants.

Plant-Air Partition Coefficients

The intermedia-transfer factors K_{pa}^{gs} and K_{pa}^{pt} , the chemical-specific plant-air partition coefficients, represent the ratio of contaminant concentration in above-ground plant parts, in mg/kg(fresh mass), to contaminant concentration in, respectively, the gas-phase of the atmosphere (gs) and particles suspended in the atmosphere (pt), both in mg/m³ (air).

For contaminants in the gas phase of the atmosphere, K_{pa}^{gs} represents the foliar-uptake and expresses the partitioning between contaminant concentration in leaf fresh mass, mg/kg, and contaminant concentration in air, mg/m³. Trapp et al.

(1990) have used barley plants in growth chambers to demonstrate that chemicals in the roots of the barley plants reach equilibrium with the soil, whereas chemicals in the shoots are in equilibrium with the air. Riederer (1990) reports that a full description of steady-state partitioning within plant foliage requires a model that includes rates of uptake from and loss to aqueous and solid phases at the surface of the cuticle and the rates of translocation, metabolism, and dilution due to growth. Riederer (1990) has shown that, for foliar uptake of gases, the most general form of a steady-state plant-air partition model is

$$K_{pa}^{gs} = \left[f_{pa} + (f_{pw} + f_{pl} \times K_{ow}) \times \frac{RT}{H} \right] \times \frac{1}{\rho_p} \quad [19]$$

where f_{pa} is the fraction of the plant tissue volume that is air; f_{pw} is the of plant tissue volume that is water; f_{pl} is the fraction of the plant tissue volume that is lipid; R is the universal gas constant, $8.31 \text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{k}$; T is the temperature, kelvins (293 K); H is the Henry's law constant in $\text{Pa}\cdot\text{m}^3/\text{mol}$; and ρ_p is the density of plant tissues in kg/m^3 . Based on azalea-leaf experiments with five chemicals, Bacci et al. (1990) have developed a correlation of leaf-air bioconcentration factors with air-water and octanol-water partition coefficients and have shown that f_{pl} is on the order of 0.01. Paterson and Mackay (1989) have estimated that f_{pa} is 0.5. This implies that the remainder of the plant volume fraction, 0.49, is either water or non-lipid solids. Based on our observation above that 80% of plant mass is water (i.e., $\text{bio}_{dm} = 0.2$), we set f_{pa} equal to 0.4. We use $1000 \text{ kg}/\text{m}^3$ as the density of plant tissue, and recommend the following expression to estimate the plant-air partition coefficient.

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} \quad [20]$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1.

Bioconcentration Factors (BCFs) in Fish

Bioconcentration factors provide a measure of chemical partitioning between a biological medium, such as fish tissue, and an external medium, such as water. The higher the BCF the more likely is partitioning to biota. The transfer of a

contaminant in water, sediment, and/or food to an aquatic organism is governed by three basic processes, namely, the uptake from the contact media, distribution to target tissue, and elimination via excretion and/or metabolic transformation. Normally, biotransfers of contaminants are measured or estimated for steady-state conditions in which intakes are equal to losses. For fish, the BCF is taken as the ratio of concentration of a xenobiotic substance in fish flesh (or lipids) to the contaminant's concentration in water (Mackay, 1982). The BCF for neutral organic compounds can be estimated from regression equations based on selected physicochemical properties, particularly a compound's K_{ow} or aqueous solubility. Mackay (1982) recommends,

$$BCF = 0.048 K_{ow} \quad [21]$$

and reports that the estimation error in this expression has a GSD of 1.8 or a CV of 0.6. Regression equations for BCFs are also discussed by Van Gestel et al. (1985) and Isnard and Lambert (1988). It should be noted that there are cases in which the measured levels of organic or inorganic substances in fish are considerably higher than the values predicted from BCF equations such as that above. This occurs as a result of bioaccumulation, which refers to the accumulation of a substance in fish from both water (i.e., bioconcentration) and the consumption of contaminated foods. Thus, a substance that bioaccumulates will usually occur at its highest concentrations in fish occupying the top trophic levels in a food chain. Generally, only those substances that are lipophilic and persistent will bioaccumulate. Models for simulating these bioaccumulation processes have been presented by Thomann (1989) and Barber et al. (1991).

Biotransfer Factors for Meat, Milk, and Eggs

The biotransfer factors B_t , B_k and B_e are the steady-state contaminant concentrations in, respectively, fresh meat, milk, and eggs divided by the animals' daily contaminant intake, and are expressed in units of (mg/kg)/(mg/d) or kg/d. Unlike bioconcentration factors, which express steady-state concentration ratios between animal tissue and a specific environmental medium, biotransfer factors express the steady-state relationship between intake and tissue or food-product concentrations. For terrestrial animals that are exposed to contaminants from multiple media (such as air, water, forage, soil, etc.), the biotransfer factor has more utility for assessing the effects of multimedia contamination on the contamination

of food. Based on a review of biotransfer factors for 28 organic chemicals in milk and 36 chemicals in meat, Travis and Arms (1988) developed the following geometric-mean regressions for B_t and B_k based on the octanol-water partition coefficient, K_{ow} ,

$$\log B_t = \log K_{ow} - 7.6 \pm 0.95 \quad (n = 36, r^2 = 0.67) \text{ and} \quad [22]$$

$$\log B_k = \log K_{ow} - 8.1 \pm 0.84 \quad (n = 28, r^2 = 0.55) . \quad [23]$$

Using the data provided by Travis and Arms (1988), we calculated the error terms, ± 0.95 and ± 0.84 , from the mean square error of the estimator for these regressions. These estimation errors correspond, respectively, to CVs of 11 and 6.

The transfer of organic chemicals from diet to food has also been expressed in terms of the fat-diet partition coefficient, K_{fd} , which is the steady-state ratio of contaminant concentration in animal fat (or lipid) to contaminant concentration in animal diet with units kg(diet)/kg(fat). Kenaga (1980b) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K_{fd} to K_{ow} ,

$$\log K_{fd} = 0.5 \log K_{ow} - 3.457 \pm 1 \quad (n = 23, r^2 = 0.62) . \quad [24]$$

The estimation error in this expression, ± 1 , was calculated by Kenaga (1980b).

There are so few measurements of diet-egg partitioning, that it is impractical at this time to develop an estimation equation. Thus, to develop a biotransfer factor for transfer of organic chemicals from chicken diet to eggs, we consider possible proxy values of K_{fd} for chickens. The correlations of Travis and Arms (1988) can be converted from biotransfer factors to fat-diet partition coefficients by multiplying the milk biotransfer factor, B_k , by the fat content of cow's milk and feed intake of dairy cattle and by multiplying the meat biotransfer factor, B_t , by the fat content of beef and feed intake of beef cattle. We did this using fat contents and feed intakes from Table IV and developed the following geometric least squared regression of K_{fd} with K_{ow} using the 64 biotransfer factors reported by Travis and Arms (1988),

$$\log K_{fd} = \log K_{ow} - 4.9 \pm 1 \quad (n = 64, r^2 = 0.61) . \quad [25]$$

For K_{ow} in the range 10^2 to 10^6 , equations [24] and [25] are within a factor of 10 of each other, which is within the range of the estimation error associated with either equation. For K_{ow} in the range 10^4 to 10^5 , equations [24] and [25] are within a factor of two of each other.

Based on measurements of polychlorodibenzodioxins (PCDDs) and polychlorodibenzofurans (PCDFs) concentrations in soil versus concentrations in egg fat and adipose tissue of foraging chickens and concentrations in the adipose tissue of grazing cattle, Stephens, et al. (1990) have shown that contaminant concentrations in animal fat correlate with soil concentrations and that the fat-soil partition factor in chicken fat is roughly six times higher than the fat-soil partition factor in cattle. However, the fraction of total intake represented by soil in the chicken diet is higher than in the cattle diet. Based on these observation and what is discussed above, we (a) assume that the fat-diet partition factor in chickens is similar to that in cattle, (b) use equation [25] to estimate the K_{fd} for chickens, and (c) use the fat content of eggs (0.08) and feed intake of chickens (0.12 kg/d [fresh mass]) to obtain the following estimate of a biotransfer factor, B_e , from chicken diet to eggs with units d/kg(eggs),

$$\log B_e = \log K_{ow} - 5.1 \pm 1 . \quad [26]$$

We estimate the CV in this expression as 14.

There are no general estimation methods for approximating the biotransfer factors of inorganic chemicals. The literature on radionuclides is often a useful source for biotransfer factors (see, for example, Ng, 1982). Stevens (1991, 1992) has reported on milk and meat biotransfer factors for toxic metals. Bowen (1979) has some limited data on transfers of elements from vegetation and soil to animal tissues.

Contaminant Biodegradation Factors in Soil

The transformation of organic and inorganic compounds by microorganisms that are present in soil can result in substantial degradation. Howard et al. (1991) have provide a review of the literature on contaminant degradation in soil due to both aerobic and anaerobic biodegradation.

Media-Specific Half Lives

A medium-specific half life provides a relative measure of the persistence of a chemical in a given medium such as soil or water. Media-specific half lives for many organic contaminants in air, soil, and surface water are summarized in Howard et al. (1991).

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PART II

INTERMEDIA TRANSFER FACTORS FOR 15 CHEMICALS

1,3-Butadiene

Other names: vinylethylene, divinyl, bivinyl, pyrrolylene, biethlylene, erythrene

CAS Registry Number: 106-99-0

1,3-butadiene is a gas at most environmental temperatures and very volatile even at low temperatures. It is produced largely from petroleum gasses by catalytic dehydrogenation of butene or butene-butane mixtures. Once released to the atmosphere, it will photooxidize by reaction primarily with hydroxyl radicals.

Formula: C₄ H₆

Molecular weight

54.09 (Weast et al., 1986; Windholz et al., 1983; Howard, 1989; Verschueren, 1983)

Melting Point

-108.9 °C (Howard, 1989; Verschueren, 1983)

Octanol-water partition coefficient (K_{ow})

97.7 derived from a log K_{ow} of 1.99 reported by Hansch and Leo (1987). This value is based on unpublished measurements carried out by Hansch and his colleagues. Also derived from a log K_{ow} of 1.99 reported in Howard(1989) based on the value published by Hansch and Leo (1985).

Recommended value:

$$\log K_{ow} = 1.99$$

$$K_{ow} = 97.7$$

Vapor pressure at standard temperatures

An extensive review of measured vapor pressures for organic compounds is reported in Stull (1947), who reports the following values for 1,3-butadiene in the range of temperatures likely to be found in the environment.

Temperature (C)	Vapor Pressure (mm)	Vapor Pressure (Pa)
-19.3	400	5.33×10^4
-4.5	760	1.01×10^5
15.3	1520	2.03×10^5
47	3800	5.07×10^5

Interpolating from this data gives VP at 25 °C = 275 kPa. These values are also given in Windholz et al. (1983).

Verschueren (1983) reports the following vapor pressures for 1,3-butadiene:

Temperature (C)	Vapor Pressure (mm)	Vapor Pressure (Pa)
-4.4	760	5.33×10^4
20	1900	2.53×10^5
30	2508	3.34×10^5

Interpolating from this data gives VP at 25 °C = 290 kPa

Wilhoit and Zwolinski (1971), Dean (1985), Boublik et al. (1984) have compiled data on vapor pressure and temperature for a number of organic compounds and have fit this data to the Antoine equation relating vapor pressure to absolute temperature for 1,3-butadiene.

$$\log_{10}(\text{VP}) = 5.975 - \frac{932}{239.3 + T} \quad , \text{ from Boublik et al. (1984), and}$$

$$\log_{10}(\text{VP}) = 5.975 - \frac{930.5}{238.9 + T} \quad , \text{ from Wilhoit and Zwolinski (1971).}$$

Both estimation equations above provide VP in kPa based on T in °C and both equations give VP = 281 kPa at 25 °C.

$$\log_{10}(\text{VP}) = 6.850 - \frac{930.5}{238.8 + T} \quad , \text{ from Dean (1985)}$$

This third equation gives VP in torr and gives VP = 2102 torr or 280 kPa at 25 °C.

The fitted Antoine equation for 1,3-butadiene from Boublik et al. (1984) is plotted below.

Recommended value:

VP = 281 kPa (2100 torr) at 25 °C

$$\log_{10}(\text{VP}) = 5.975 - \frac{932}{239.3 + T} \text{ kPa in the range } -10 \text{ to } 40\text{ }^{\circ}\text{C}$$

Solubility in water

735 mg/L at 25°C measured and reported by McAuliffe (1966)

735 mg/L at 20 °C reported by Verschueren (1983)

735 mg/L at 25 °C reported by Howard (1989), who attributes this value to McAuliffe (1966).

600 mg/L at 38 °C as interpolated from the measured data of Reed and McKetta (1959).

Recommended value:

WS = 735 mg/L at 25 °C

Henry's law constant

- 2.57 dimensionless Henry's law constant ($\{\text{mol/L[air]}\}/\{\text{mol/L[water]}\}$) reported in Howard (1989) based on a value reported in Hine and Mookerjee (1975). However, there appears to be an error in the reported value of $\log H$ reported in Hine and Mookerjee (1974). They report the log of the equilibrium air concentration, $\log c_g$, as -1.39 and the log of the equilibrium water concentration, $\log c_w$ as -1.87 (which corresponds to a water solubility of 730 mg/L). They report $\log (H/RT)$, the difference, $\log c_g - \log c_w$, as 0.41 (corresponding to $H/RT = 2.57$) when it is actually 0.48 (corresponding to $H/RT = 3.02$).
- 3.02 at 25°C based on the actual values for vapor pressure and solubility reported in Hine and Mookerjee (1975) (and not on the reported ratio). This value is also obtained from ratio of VP to WS values reported above. Shown below is the estimated variation of the dimensionless Henry's law constant versus temperature for 1,3-butadiene. It should be noted that the vapor pressure of 1,3-butadiene cannot exceed atmospheric pressure in the air above a water solution.

Recommended dimensionless value:

$$H/RT = 3.02 \text{ @ } 25^\circ\text{C}$$

Organic-carbon partition coefficient (K_{oc})

No reported measurements of K_{oc} or K_d for 1,3-butadiene in soils or sediments are available in the current literature. Estimation methods for K_{oc} produce the following values for K_{oc} ,

283 as derived from the K_{oc} estimation method proposed by Kenaga and Goring (1980) and referred to in Lyman et al. (1990)

83.7, 73.7, 41.9, and 47 as derived from the four regression equations relating K_{oc} to K_{ow} in Karickhoff (1985).

112 as derived from the regression of K_{oc} with solubility proposed by Chiou et al. (1977)

116 as derived from the regression of K_{oc} with solubility proposed by Kenaga (1980)

162 as derived from the regression of K_{oc} with the molecular connectivity index ($^1\chi = 3$) as proposed by Meylan et al (1992).

Recommended value based on the log mean of the predicted values above:

$$\log K_{oc} = 2.0 \pm 0.25$$

$$K_{oc} = 100 \times \text{or} \div 1.8$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}} .$$

The molecular weight, M_y , of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 1.0 cP at 20 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With the molecular volume V_x of 1,2-butadiene equal to 77.9 cm^3/mol , this expression gives

$$D_{\text{water}} = 3.7 \times 10^{-7} T \text{ m}^2/\text{d} = 1.1 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.3 \times 10^{-9} \text{ m}^2/\text{s} @ 293\text{K}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2} .$$

With the molecular volume, V_x , of 1,3-butadiene equal to $77.9 \text{ cm}^3/\text{mol}$ and a molecular weight of 54.09 g/mol , the above expression gives

$$D_{\text{air}} = 4.7 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.84 \text{ m}^2/\text{d} \text{ or } 9.8 \times 10^{-6} \text{ m}^2/\text{s} @ 293\text{K}$$

Bioconcentration factors for plant tissue concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for 1,3-butadiene in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, $K_{\text{ps}}^{\text{rain}}$ is equal to $0.0034 \text{ kg(soil)/kg(plant)}$ with a CV of 1 (Dreicer et al. 1984). This partition factor relates plant fresh mass concentration to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, $\text{mg/kg}[\text{fresh mass}]$, to contaminant concentration in soil solution, mg/L) for 1,3-butadiene as

$$\text{RCF} = 1.84$$

When this factor is divided by the sorption coefficient, $K_d = f_{\text{oc}} \times K_{\text{oc}} = (0.01 \text{ to } 0.02) \times K_{\text{oc}}$ (from above), we obtain the ratio of contaminant concentration in roots, $\text{mg/kg}(\text{fresh mass})$ to contaminant concentration in soil solids, mg/kg , which we refer to as $K_{\text{ps}}(\text{roots})$ and estimate it as being in the range

$$K_{ps}(\text{roots}) = 0.32 \text{ to } 4.4$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

$$K_{ps}(\text{roots}) = 4.5 \text{ to } 15 \text{ (recommended range for root crops)}$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient.

$$K_{ps} = 0.54 \times \text{or} + 5.4 \text{ (recommended value for exposed produce)}$$

Bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for 1,3-butadiene in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 0.63 \text{ (recommended value)}$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

No information on the bioconcentration factor for 1,3-butadiene could be found in the literature. However, based our recommended K_{ow} value, we estimate bioconcentration factor (BCF) is 4.6 based on the correlation of Mackay (1982). Howard (1989) reports a bioconcentration factor estimated from K_{ow} of 19.

$$\text{BCF} = 4.6 \text{ (recommended value)}$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for 1,3-butadiene are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988), we estimate the milk biotransfer factor for 1,3-butadiene as

$$\log B_k = -6.1 \pm 0.84 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for 1,3-butadiene are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for 1,3-butadiene as

$$\log B_t = -5.6 \pm 0.95 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for 1,3-butadiene are available in the current literature. An estimation method value for this parameter is considered below.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for 1,3-butadiene as

$$\log B_e = -3.1 \pm 1 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Howard et al. (1991) have estimated the half-life of 1,3-butadiene in soil due to aerobic biodegradation to be in the range of 7 to 28 days.

Recommended value, based on log mean and log variance of the range of the soil half lives given above:

$$\text{Soil biodegradation rate constant} = 0.05 \text{ d}^{-1} \times \text{or} \pm 1.5$$

Media-specific half lives for air, soil, and surface water

Air. Howard et al. (1991) estimate the half life of 1,3-butadiene in lower atmosphere is in the range of 1 to 8 hours (0.042 to 0.33 days) and that removal from air is due primarily to reaction with hydroxyl radicals.

Soil Howard et al. (1991) have estimated the half-life of 1,3-butadiene in soil due to aerobic biodegradation to be in the range of 7 to 28 days.

Water. When released to water, 1,3-butadiene evaporates rapidly with a half life estimated to be several hours; it does not hydrolyze appreciably, but may be subject to some biodegradation (Howard et al., 1991).

Recommended half-lives (in days), based on the log mean of the half lives and geometric range of the values:

Air $0.12 \times \text{or} \pm 1.8$

Soil $14 \times \text{or} \pm 3.5$

Water $0.12 \times \text{or} \pm 1.5$

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Cadmium (Cd)

Cadmium typically occurs in nature in association with zinc ores, such as sphalerite (ZnS). Greenockite (CdS) is the only mineral of any consequence bearing cadmium (Weast et al., 1986). Almost all cadmium used industrially is obtained as a by-product in the treatment of zinc, copper, and lead ores. Cadmium has a only one valence state, +2. Cadmium forms a number of salts, including cadmium chloride (CdCl₂), cadmium sulfate (CdSO₄), and cadmium sulfide (CdS). Cadmium sulfate is the most common salt. Cadmium has a relatively high bioavailability. It is accumulated and retained in the human body.

Molecular and atomic weights

- 112.41 g/mol, atomic weight of Cd (Weast et al., 1986).
- 112.4 g/mol, atomic weight of Cd (Bowen, 1979).
- 183.32 g/mol, molecular weight of cadmium chloride, CdCl₂ (Weast et al., 1986).
- 208.47 g/mol, molecular weight of cadmium sulfate, CdSO₄ (Weast et al., 1986).
- 144.47 g/mol, molecular weight of cadmium sulfide, CdS (Weast et al., 1986).

Melting points

- 321 °C for cadmium metal, Cd (Stull, 1947).
- 568 °C for cadmium chloride, CdCl₂ (Stull, 1947).
- 1000 °C for cadmium sulfate, CdSO₄ (Weast et al., 1986).
- cadmium sulfide, CdS, boils before it melts (Weast et al., 1986).

Vapor pressure

- 765 °C is the boiling point of pure cadmium, Cd (Stull, 1947).
- 967 °C is the boiling point of cadmium chloride, CdCl₂, reported by Stull (1947).
- 960 °C is the boiling point of cadmium chloride, CdCl₂, reported by (Weast et al., 1986).
- 980 °C is the boiling point of cadmium sulfide, CdS, reported by (Weast et al., 1986).

Stull (1947) reports the following vapor pressures for cadmium metal (Cd).

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
394	1	0.133
455	5	0.667
484	10	1.33
516	20	2.67
553	40	5.33
578	60	8.00
611	100	13.3
658	200	26.7
711	400	53.3
765	760	101

Interpolating from this data using an Antoine equation gives
VP at 25 °C = 1.7×10^{-8} Pa

Stull (1947) reports the following vapor pressures for cadmium chloride (CdCl₂).

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
618	5	0.667
656	10	1.33
695	20	2.67
736	40	5.33
762	60	8.00
797	100	13.3
847	200	26.7
908	400	53.3
967	760	101

Interpolating from this data using an Antoine equation gives
VP at 25 °C = 0.95 Pa

Recommended value:

No recommended vapor pressure for cadmium
because the speciation of its compounds makes vapor pressure
unimportant for characterizing environmental transport

Solubility in water

In aqueous systems, water hardness along with pH determine the speciation of cadmium. In fresh water at typical environmental pH values of 6 to 8, Cd^{+2} is the predominant species (Bodek et al., 1988). The only oxidation state of importance for cadmium under environmental conditions is +2. In the presence of sulfide ions and under reducing conditions, cadmium sulfide is formed over a wide pH range. The resulting precipitation of cadmium sulfide in reducing environments can serve to control the effective solubility of cadmium in natural waters.

metal cadmium, Cd, is insoluble in water (Weast et al., 1986).

1,680,000 mg/L (9170 mol/m³) of cadmium chloride (CdCl_2), at 20 °C (Weast et al., 1986).

2,160,000 mg/L (11,790 mol/m³) of cadmium chloride (CdCl_2), at 100 °C (Weast et al., 1986).

755,000 mg/L (3620 mol/m³) of cadmium sulfate (CdSO_4), at 0 °C (Weast et al., 1986).

608,000 g/L (2920 mol/m³) of cadmium sulfate (CdSO_4), at 100 °C (Weast et al., 1986).

1.3 mg/L (9.0 mol/m³) of cadmium sulfide (CdS), at 18 °C (Weast et al., 1986).

Recommended values:

$\text{WS}(\text{Cd metal}) = \sim 0$

$\text{WS}(\text{Cd}^{+2}) = 9 \text{ to } 12,000 \text{ mol/m}^3$ depending on the presence of sulfate and sulfide ions and the Eh of the water.

Henry's law constant

Because of their almost complete speciation in water and extremely low vapor pressures, most cadmium compounds do not have measurable or predicted Henry's law constants. However, at low concentrations, the ratio of air to water concentration in air and water environments that are in contact can be estimated as

$$C_w/C_a = A \times v_d / (V_w \times R_w)$$

where C_w is the cadmium concentration in a given water body, mol/m³; C_a is the cadmium concentration in air above the water body, mol/m³; v_d is the

deposition velocity that represents the rate of cadmium transfer from air to water, m/d; A is the contact area between the air and water, m^2 ; V_w is the volume of the water body, m^3 ; and R_w is the first-order rate constant that accounts for all cadmium removals from water (i.e. precipitation and deposition), day^{-1} .

Partition coefficients in soils and sediments

1.2 -2.5 L/kg reported by Bodek et al. (1988) as the range of K_d values observed for Cd in sediments.

Bodek et al. (1988) list ranges of Freundlich isotherms parameters for modeling sorption of cadmium in four different soil types. The following Freundlich-isotherm derived distribution coefficients, K_d , bracket the range of isotherms developed by Bodek et al. (1988),

$$K_d = S/C = 0.63 C^{0.95}/C \text{ [L/kg]}$$

$$K_d = S/C = 23.2 C^{0.63}/C \text{ [L/kg]}$$

where S is the sorbed cadmium concentration, mg/kg, and C is cadmium concentration in water, mg/L. The solid lines in the figure below illustrate the dependence of the distribution coefficient for cadmium on cadmium concentration in the water phase based on these Freundlich isotherms.

Bodek et al. (1988) also list ranges of Langmuir constants for cadmium in sediments. These equations give the following estimates of the distribution coefficient K_d in river sediments.

$$K_d = S/C = A_m K_L / (1 + K_L C) \text{ [L/kg]}$$

where

S is the cadmium sorbed to soil, mol/kg;

C is the cadmium concentration in sediment water, mol/L;

A_m is the maximum amount of cadmium that can be absorbed by soil and ranges from 0.002 to 0.17 mol/kg for sediments; and

K_L is the measure of bond strength holding the sorbed cadmium to the soil surface and ranges from 25,000 to 10^7 L/mol for sediments.

The two dotted lines in the figure below represent this range of distribution coefficients associated with the range of Langmuir constants quoted above for sediments.

Recommended value of K_d for cadmium in soils and in sediments based on the geometric mean and geometric standard deviation of values considered above:

$$1 \leq K_d \leq 9,000 \text{ in soils}$$

$$200 \leq K_d \leq 160,000 \text{ in sediments}$$

$$\log K_d = 2.00 \pm 1.1 \text{ in soils}$$

$$\log K_d = 3.75 \pm 0.83 \text{ in sediments}$$

$$K_d = 200 \times \text{ or } + 12.6 \text{ in soils}$$

$$K_d = 5600 \times \text{ or } + 6.9 \text{ in sediments}$$

Diffusion coefficient in water

In dilute solutions of ionized species, such as cadmium compounds, in which there are no rapid chemical reactions and the solution is isothermal, Bodek et al. (1988) have shown that diffusion coefficients for the anions and cations in solution do not vary greatly and are on the order of $1.5 \times 10^{-9} \text{ m}^2/\text{s}$. The

diffusion coefficients of many simple salts generally do not vary by more than a factor of 2 over a range of concentrations and temperatures even though their conductivities can vary greatly (Bodek et al., 1988).

Recommended value:

$$D_{\text{water}} = 1.3 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.5 \times 10^{-9} \text{ m}^2/\text{s} \times \text{or} + 2 \text{ for } 0^\circ\text{C} \leq T \leq 40^\circ\text{C}$$

Diffusion coefficient in air

Because of the extremely low vapor pressure of cadmium and inorganic cadmium compounds, these chemical species are not likely to be found in the gas phase of the environment. There is no need for a diffusion coefficient in air and, thus no value is recommended.

Bioconcentration factors for plant tissue relative to soil concentration kg(soil)/kg(plant fresh mass), K_{ps}

Cadmium is considered a potential essential trace element for plants and animals (Mertz, 1981). Root uptake of cadmium as Cd^{+2} in plants is passive and occurs through uptake by roots of Cd dissolved in water; cadmium is highly mobile in plants and readily translocated to other plant parts (Bodek et al. (1988).

0.055 to 0.17 based on a soil-to-plant-dry-mass coefficient of 0.55 used by Baes et al. (1984) for the vegetative portion of food crops and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.015 to 0.045 based on soil-to-plant-dry-mass coefficient of 0.15 used by Baes et al. (1984) for the non-vegetative (reproductive) portion of food crops and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

0.029 to 2.1 based on a 0.35 mg/kg as the geosphere average of soil cadmium concentration and 0.1 to 2.4 mg/kg (dry mass) as a geosphere average of land-plant cadmium concentration reported by Bowen (1979) and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

$0.5 \times \text{or} + 9$ based on a 0.01 to 1 mg/kg as the range of background soil cadmium levels and 0.1 to 0.8 mg/kg (dry mass) as the range of background soil plant levels reported by Bodek et al. (1988) and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

$0.0034 \times \text{or} + 2.2$ is the partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} (Dreicer et al. 1984).

Recommended value of K_{ps} based on the log mean of the ranges of values considered above (excluding rainsplash),

$$\log K_{ps} = -0.88 \pm 0.89$$

$$K_{ps} = 0.13 (\times \text{ or } + 7.8) \text{ kg(soil)/kg(plant fresh mass)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

According to Bodek et al. (1988), airborne deposition is believed to contribute to concentrations of cadmium found in plant leaves. At low concentrations, the ratio of plant leaf concentration to air concentration when air and plant environments are in contact, can be estimated as

$$C_p/C_a = A \times v_d / (V_p \times R_p)$$

where C_p is cadmium concentration in the plants in contact with contaminated air, mol/m³; C_a is the cadmium concentration in air above the plants, mol/m³; v_d is the deposition velocity that represents the rate of cadmium transfer from air to plant surfaces, m/d; A is the contact area between the air and plants, m²; V_p is the volume of the plants compartment, m³; and R_p is the first-order rate constant that accounts for all cadmium removals from plants (i.e. wash-off, biodegradation, etc.), day⁻¹.

Bioconcentration factors for fish concentration relative to water or sediment concentrations

- 50,000 reported by Bodek et al. (1988) as a typical concentration ratio in marine invertebrates relative to water concentration.
- 3,000 reported by Bodek et al. (1988) as a typical concentration ratio in marine fish relative to water concentration.
- 2,000 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater invertebrates relative to water concentration.
- 200 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater fish relative to water concentration.
- 200 to 6000 based on 0.0001 mg/L as a geosphere average of ocean-water cadmium concentration and 0.1 to 3 mg/kg (dry mass) as an average of marine-fish cadmium concentration reported by Bowen (1979) and our assumed fish dry mass fraction of 0.2.

Recommended BCF value, based on the geometric mean and geometric standard deviation reflecting the range of BCF values described above:

$$\log \text{BCF}(\text{fish}) = 3.3 \pm 0.91$$

$$\text{BCF}(\text{fish}) = 2000 \times \text{or} + 8.1$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle, B_k

1.5×10^{-3} d/L is uptake to milk from feed based on radioisotope studies reported by Ng (1982).

Stevens (1991) evaluated several studies investigating the concentration of soluble forms of cadmium (Cd) in milk relative to the Cd intake in feed.

0.56 to 6.3×10^{-6} d/L is the range of values Stevens (1991) identified in studies investigating the concentration of soluble forms of cadmium (Cd) in milk, relative to the Cd intake in feed.

1.3×10^{-6} d/L was derived from a study by Vreman et al. (1986) by Stevens (1991) who recommended this estimate of this biotransfer factor.

Recommended biotransfer factor, B_k , for milk based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_k = -5.0 \pm 1.5$$

$$B_k = 5 \times 10^{-5} \times \text{or} + 32$$

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

Stevens (1992) evaluated several studies investigating the concentration of soluble forms of cadmium (Cd) in meat from cattle, relative to the Cd intake in feed by these cattle.

1 to 10×10^{-4} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of cadmium (Cd) in bovine muscle relative to the Cd intake in feed.

7.7 to 48×10^{-3} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of cadmium (Cd) in bovine kidney relative to the Cd intake in feed.

4.7 to 19×10^{-2} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of cadmium (Cd) in bovine liver relative to the Cd intake in feed.

1.7×10^{-4} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for cadmium to bovine muscle.

4.8×10^{-2} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for cadmium to bovine liver.

1.9×10^{-1} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for cadmium to bovine kidney.

Recommended biotransfer factor, B_t , for meat based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_t = -2.00 \pm 1.26$$

$$B_t = 0.01 \times \text{or} + 18$$

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for cadmium are available in the current literature.

Ng (1982) has shown that for the seven elements strontium, rubidium, iodine, cesium, cerium, plutonium, and americium, the ratio of egg contents biotransfer to beef biotransfer is $60 \times \text{or} + 13$. Based on this observation, the meat biotransfer above can be used to make an estimate of egg contents biotransfer of $0.6 \times \text{or} + 19$ where the larger GSD mostly reflects the uncertainty in the meat biotransfer factor.

Recommended biotransfer factor, B_e , for eggs:

$$\log B_e = -0.22 \pm 1.28$$

$$B_e = 0.6 \times \text{or} + 19$$

Contaminant biodegradation factors in soil

There is no evidence of biodegradation of inorganic cadmium in soils and sediments (Bodek et al. 1988). Thus, there is no recommended biodegradation factor for inorganic cadmium compounds in soils.

Media-specific half lives for air, soil, and surface water

There is no evidence that inorganic cadmium compounds react in air, soil, or water in such a way as to increase an existing physical removal of cadmium from these compartments. Thus the half lives of cadmium species in these compartments will depend entirely upon the removal rate due to natural physical processes such as deposition and erosion.

Recommended half-lives:

<i>Air</i>	deposition half life
<i>Soil</i>	erosion half life
<i>Water</i>	suspended particle half life

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Cellosolve

Other names: Ethylene glycol monoethyl ether, ethoxol, ethylglycol, glycolmonoethylether, 2-ethoxyetanol, Dowanol EE, Jeffersol EE, Oxitol, Ethyl cellosolve.

CAS Registry Number: 110-80-5

Cellosolve is released into the atmosphere as a result of its use as a evaporative solvent in the preparation of a variety of products. Approximately 50% of cellosolve produced is utilized for cellosolve acetate production (IPCS, 1990). It is used as a solvent for nitrocellulose; for natural and synthetic resins for surface coatings; and for dyes in textile and leather finishing. It is also used as a general solvent in varnish removers and cleansing solutions. Cellosolve is used in dry cleaning compounds and as a solvent in ink formulations for printing, photographic and photolithographic processes (Windholz et al., 1983; Howard et al., 1990; Verschueren, 1983).

Formula: $C_4H_{10}O_2$

Molecular weight

90.12 (Howard et al., 1990)

90.1 (Verschueren, 1983; Weast et al., 1986; Windholz et al., 1983)

Recommended molecular weight for cellosolve: 90.1

Melting Point

not available

Octanol-water partition coefficient (K_{ow})

0.288 derived from a log K_{ow} of -0.54 reported by Hansch and Leo (1987) based on the value measured by Collander (1951).

- 0.288 derived from a log K_{ow} of -0.54 reported by Verschueren (1983) and apparently taken from an earlier edition of Hansch and Leo (1987).
- 0.447 derived from a log K_{ow} of -0.35 reported by Hansch and Leo (1987) based on the measured value they attribute to Funasaki et al. (1984).
- 0.794 derived from a log K_{ow} of -0.10 reported by Hansch and Leo (1987) based on the value measured by Korenman and Udalova (1974) [This value is also cited by Howard (1990).

Recommended value, based on the log-mean value of the 3 measured values reported above:

$$\log K_{ow} = -0.33 \pm 0.22$$

$$K_{ow} = 0.47 \times \text{or} \div 1.6$$

Vapor pressure at standard temperatures

- 0.507 Pa based on a VP of 3.8 mm Hg at 20 °C reported in IPCS (1990) attributed to Rowe and Wolf (1982).
- 0.707 Pa based on a VP of 5.3 mm Hg at 25 °C reported in Howard et al. (1990) and attributed to the Dow Chemical Company Glycol Ethers Handbook (1981).
- 0.767 Pa based on a VP of 5.75 mm Hg at 25 °C reported in Rowe and Wolf (1982).
- 0.933 Pa based on a VP of 7 mm Hg at 30 °C reported in Verschueren (1983).

The following Antoine equation has been published for estimating the vapor pressure of cellosolve in kPa

$$\log_{10} (\text{VP in kPa}) = 6.972 - \frac{1825}{232.483 + T} \quad \text{for } 63^\circ\text{C} < T < 134^\circ\text{C} \quad \text{from Boublik et al. (1984),}$$

which gives VP(kPa) = 0.765 = at 25°C.

The Antoine equation above proposed by Boublik et al. (1984) for VP versus temperature is plotted below in the temperature range -10 °C < T < 40 °C.

Recommended value for the temperature range -10 to 40 °C, based on the Antoine equation of Boublik et al. (1984) above:

$$VP(kPa) = 10^{[6.972 - 1825/(232.483 + T)]} \pm 0.?? \text{ for } -10\text{ °C} < T < 40\text{ °C}$$

Recommended value at 25 °C, based on the mean of the three values above:

$$VP(kPa) = 0.75 \pm 0.034 \text{ @ } 25\text{ °C}$$

Solubility in water

Miscible with water (Howard et al., 1990; Rowe and Wolf, 1982).

Henry's law constant (dimensionless form)

- 2.1 based on $5.2 \times 10^3 \text{ Pa} \cdot \text{m}^3/\text{mole}$ (or $5.13 \times 10^3 \text{ atm} \cdot \text{m}^3/\text{mole}$) reported by Howard et al. (1990).

Organic-carbon partition coefficient (K_{oc})

No reported measurements of K_{oc} or K_d for cellosolve in soils or sediments are available in the current literature. With $K_{ow} = 0.47$, estimation methods for K_{oc} produce the following values for K_{oc} ,

16 as derived from the regression equation relating K_{oc} to K_{ow} in Kenaga and Goring (1980) and referred to in Lyman et al. (1990).

1.8, 0.30, 0.21, and 0.23 as derived from the four regression equations relating K_{oc} to K_{ow} in Karickhoff (1985).

1.8 as derived from the regression as proposed by Meylan et al (1992) of K_{oc} with the molecular connectivity index ($^1\chi = 2.91$) and a correction factor of -2.528 for the aliphatic-ether and aliphatic-alcohol C—O bonds.

Recommended value, based on the log-mean value of the 6 values reported above:

$$\log K_{oc} = -0.02 \pm 0.74$$

$$K_{oc} = 0.95 \times \text{ or } \div 5.5$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}}$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). With the molecular volume V_x cellosolve equal to 101 cm^3/mol , this expression gives

Recommended value:

$$D_{\text{water}} = 3.1 \times 10^{-7} T \text{ m}^2/\text{d} = 9.3 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 1.0 \times 10^{-9} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of cellosolve of $101 \text{ cm}^3/\text{mol}$ and a molecular weight of 90.1 g/mol , the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 3.4 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.73 \text{ m}^2/\text{d} \text{ or } 8.4 \times 10^{-6} \text{ m}^2/\text{s} @ 25^\circ\text{C}$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, $K_{\text{ps}}^{\text{rain}}$ is equal to $0.0034 \text{ kg}(\text{soil})/\text{kg}(\text{plant})$ with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, $\text{mg}/\text{kg}[\text{fresh mass}]$, to contaminant concentration in soil solution, mg/L) for cellosolve as

$$\text{RCF} = 0.82 + 0.03 K_{\text{ow}}^{0.77} = 0.84$$

When this factor is divided by the sorption coefficient, $K_d = f_{\text{oc}} \times K_{\text{oc}} = (0.01 \text{ to } 0.02) \times K_{\text{oc}}$ (from above), we obtain the ratio of contaminant concentration in roots, $\text{mg}/\text{kg}(\text{fresh mass})$ to contaminant concentration in soil solids, mg/kg , which we refer to as $K_{\text{ps}}(\text{roots})$ and estimate it as being in the range

$$K_{\text{ps}}(\text{roots}) = 44 \text{ to } 88 \times \text{ or } \div 5.5 \text{ (reflecting the error in } K_{\text{oc}})$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

(recommended range for root crops)

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 685 \times \text{or} + 5.5 \text{ (reflecting the error in } K_{oc}\text{)}$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 12 \times \text{or} + 1.6 \text{ (recommended value for exposed produce reflecting the error in } K_{ow}\text{)}$$

Bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for cellosolve in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 0.0013 \text{ (recommended value)}$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1 (or GSD=2.3).

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

No information on the bioconcentration factor for cellosolve could be found in the literature. However, based on its K_{ow} value, its estimated bioconcentration factor is 0.02 based on the correlation of Mackay (1982).

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for cellosolve are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for cellosolve as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 3.7 \times 10^{-9} \times \text{or} + 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for cellosolve are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for cellosolve as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 1.2 \times 10^{-8} \times \text{or} + 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for cellosolve are available in the current literature. An estimation method value for this parameter is considered below.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for cellosolve as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 3.7 \times 10^{-6} \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Based on experiments by Bogan and Sawyer (1955) Howard et al. (1991) have estimated the half-life of cellosolve in soil due to aerobic biodegradation to be in the range of 7 to 28 days.

Recommended value, based on log mean and log variance of the range of the soil half lives given above:

$$\text{Soil biodegradation rate constant} = 0.05 \text{ d}^{-1} \times \text{or} + 1.5$$

Media-specific half lives for air, soil, and surface water

- Air.* Based on measurements of the photooxidation half-life in air by Atkinson (1987), Howard et al. (1991) estimate the half life of cellosolve in the lower atmosphere to be in the range 5.4 to 54 hours (0.23 to 2.3 days) with removal from air is due primarily to reaction with hydroxyl radicals and nitrogen dioxides.
- Soil* Howard et al. (1991) have estimated that cellosolve is not expected to bound to soil tightly. It is expected to leach to ground water and volatilize. Biodegradation may be significant. Their estimate of its half-life in soil is in the range 7 to 28 days due primarily to biodegradation.
- Water.* When released to water, cellosolve volatilizes rapidly with no estimation of half-life. It may be subject to significant biodegradation (Howard et al., 1991). Its photooxidation half-life in water is on the order of years. Based on aerobic biodegradation, (Howard et al., 1991) estimate the half-life of cellosolve in surface water to be in the range of 7 to 28 days.

Recommended half-lives (in days), based on the log mean of the half lives and geometric range of the values:

Air $0.73 \times \text{or} + 1.9 \text{ days}$

Soil $14 \times \text{or} + 3.5 \text{ days}$

Water $14 \times \text{or} + 3.5 \text{ days}$

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Cellosolve Acetate

Other names: Ethoxyethyl acetate, B-ethoxyethyl acetate, 2-ethoxyethyl acetate, ethyl cellosolve acetate, ethylene glycol ethyl ether acetate, ethylene glycol monoethyl ether acetate, glycol monoethyl ether acetate, oxytol acetate, poly-solve EE.

CAS Registry Number: 111-15-9

Cellosolve acetate is directly released into the atmosphere through its use as a solvent for surface coatings (especially the epoxy-resins based ones). It is also used as a solvent in cleaning and printing ink formulations, in coating applications for automobile, coils, machinery and equipment, and metal furniture and appliances.

Formula: $C_6H_{12}O_3$

Molecular weight

132.16 (Howard et al., 1993; Windholz et al., 1983)

Recommended molecular weight for cellosolve acetate: 132.2
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Melting Point

-61.7 °C (Howard et al., 1993)

Octanol-water partition coefficient (K_{ow})

3.16 derived from a log K_{ow} of 0.5 reported by Montgomery (1991) based on the methods of Leo et al. (1971).

4.47 derived from a log K_{ow} of 0.65 reported by Howard (1993) based on the value estimated using the U.S. Environmental Protection Agency computer program CLOPG with in the Graphical Exposure Modeling System (GEMS), 1986 version.

Recommended value, based on the log-mean value of the 2 values reported above:

$$\log K_{ow} = 0.58 \pm 0.11$$

$$Kow = 3.8 \times 10^{+1.3}$$

Vapor pressure at standard temperatures

- 159.9 Pa based on a VP of 1.2 mm Hg at 20 °C reported by Montgomery (1991) based value reported by Sax and Lewis (1987).
- 159.9 Pa based on a VP of 1.2 mm Hg at 20 °C reported in Verschueren (1983).
- 159.9 Pa based on a VP of 1.2 mm Hg at 20 °C reported by Rowe and Wolf (1982).
- 219.9 Pa based on a VP of 1.65 mm Hg at 20 °C reported in Howard et al. (1993) and attributed to Daubert and Danner (1989).
- 266.6 Pa based on a VP of 2 mm Hg at 20 °C reported by Montgomery (1991) based a report from NIOSH (1987).
- 373.2 Pa based on a VP of 2.8 mm Hg at 25 °C reported by Rowe and Wolf (1982).
- 506.6 Pa based on a VP of 3.8 mm Hg at 30 °C reported by Verschueren(1983).
- 101,324 Pa based on the boiling point of 156 °C reported by Howard (1993).

The values reported above were fit to an Antoine equation in order to interpolate the vapor pressure of cellosolve acetate at environmental temperatures in the range -10 to 40 °C. The results of this fit are plotted below. This curve gives VP = 282 Pa at 25 °C.

Recommended vapor pressure based on the Antoine equation interpolation from the data above:

$$VP = 282 \pm 65 \text{ Pa @ } 25^\circ \text{ C}$$

Solubility in water

229,000 mg/L at 20 °C reported by Howard et al (1993), based on a value reported by Riddick et al. (1984)

142,857 mg/L based on solubility of 1 in 6 parts of water at an unspecified temperature reported by the Merck Index (Windholz et al. 1983).

Recommended solubility based on the mean range and variance of the 2 values reported above:

$$WS = 185,000 \pm 25,000 \text{ mg/L}$$

Henry's law constant (dimensionless form)

5.4×10^{-5} based on $1.3 \times 10^{-1} \text{ Pa} \cdot \text{m}^3/\text{mole}$ (or $1.25 \times 10^{-6} \text{ atm} \cdot \text{m}^3/\text{mole}$) at 20 °C calculated from the ratio of vapor pressure to solubility by Howard et al. (1993).

3.8×10^{-5} based on $9.2 \times 10^{-2} \text{ Pa} \cdot \text{m}^3/\text{mole}$ (or $9.07 \times 10^{-7} \text{ atm} \cdot \text{m}^3/\text{mole}$) at 20 °C reported by Montgomery (1991).

$8.1 (\pm 2.2) \times 10^{-5}$ at 25 °C based on the mean and standard deviation of vapor pressure and solubility recommended above and the variance propagation in the expression $H = VP/(WS R T)$.

Recommended Henry's law value based on the H value calculated above at 25 °C:

$$H/(RT) = 8.1 (\pm 2.2) \times 10^{-5} \text{ at } 25^\circ\text{C}$$

Organic-carbon partition coefficient (K_{oc})

No reported measurements of K_{oc} or K_d for cellosolve acetate in soils or sediments are available in the current literature. With $K_{ow} = 3.8$ ($\log K_{ow} = 0.58$) and $WS = 185,000 \text{ mg/L}$, estimation methods for K_{oc} produce the following values for K_{oc} ,

- 49 as derived from the regression equation relating K_{oc} to K_{ow} in Kenaga and Goring (1980) and referred to in Lyman et al. (1990).
- 8.1, 3.7, 1.7, and 1.8 as derived from the four regression equations relating K_{oc} to K_{ow} in Karickhoff (1985).
- 7.1 as derived from the regression of K_{oc} with water solubility proposed by Chiou et al. (1977)
- 5.5 as derived from the regression of K_{oc} with water solubility proposed by Kenaga (1980)
- 2.4 as derived from the regression as proposed by Meylan et al (1992) of K_{oc} with the molecular connectivity index ($^1\chi = 4.4$) and a correction factor of -2.573 for the one aliphatic-ether and one aliphatic-ester C-O bonds .

Recommended value, based on the log-mean value of the 8 values reported above:

$$\log K_{oc} = 0.70 \pm 0.48$$

$$K_{oc} = 5.0 \times \text{ or } \div 3.0$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}} .$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). With the molecular volume V_x cellosolve acetate equal to 163 cm³/mol, this expression gives

Recommended value:

$$D_{\text{water}} = 2.4 \times 10^{-7} T \text{ m}^2/\text{d} = 7.0 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 8.1 \times 10^{-10} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m²/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of cellosolve acetate of 163 cm³/mol and a molecular weight of 132.2 g/mol, the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 2.6 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.57 \text{ m}^2/\text{d} \text{ or } 6.5 \times 10^{-6} \text{ m}^2/\text{s} \text{ at } 25 \text{ }^\circ\text{C}$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, $K_{\text{ps}}^{\text{rain}}$ is equal to 0.0034 kg(soil)/kg(plant) with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, mg/kg[*fresh mass*], to contaminant concentration in soil solution, mg/L) for cellosolve acetate as

$$\text{RCF} = 0.82 + 0.03 K_{ow}^{0.77} = 0.90$$

When this factor is divided by the sorption coefficient, $K_d = f_{oc} \times K_{oc} = (0.01 \text{ to } 0.02) \times K_{oc}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg(*fresh mass*) to contaminant concentration in soil solids, mg/kg, which we refer to as $K_{ps}(\text{roots})$ and estimate it as being in the range

$$K_{ps}(\text{roots}) = 9.0 \text{ to } 18 \times \text{or} \pm 3 \text{ (reflecting the error in } K_{oc})$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

(recommended range for root crops)

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 240 \times \text{or} \pm 3 \text{ (reflecting the error in } K_{oc})$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 3.5 \times \text{or} \pm 5.4 \text{ (recommended value for exposed produce reflecting the error in } K_{ow})$$

Bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for cellosolve acetate in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 5.4 \text{ (recommended value)}$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1 (or GSD=2.3).

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

No information on the bioconcentration factor for cellosolve acetate could be found in the literature. However, based on its K_{ow} value, its estimated bioconcentration factor is 0.182 based on the correlation of Mackay (1982). This value is so low as to indicate no bioconcentration. No BCF other than unity is recommended

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for cellosolve acetate are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for cellosolve acetate as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 3.0 \times 10^{-8} \times \text{or} \div 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for cellosolve acetate are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for 1,3-butadiene as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 9.5 \times 10^{-8} \times \text{or} \div 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for cellosolve acetate are available in the current literature. An estimation method value for this parameter is considered below.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for cellosolve acetate as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 3.0 \times 10^{-5} \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Howard et al. (1993) report that cellosolve acetate is readily biodegradable in soils. They indicate that its half-life in soil is on the order of days. However, since there is a lack of substantive data on biodegradation, we provide here no recommended value.

Media-specific half lives for air, soil, and surface water

Air. Howard et al. (1993) estimate the half life of cellosolve acetate in lower atmosphere is on the order of about 1.2 days due primarily to photo-chemical reaction with hydroxyl radicals.

Soil Howard et al. (1993) report that cellosolve acetate is readily biodegradable in soils with half-life in soil is on the order of days. Since there is a lack of substantive data on biodegradation, we provide here no recommended value.

Water. Howard et al. (1993) report that cellosolve acetate is also readily biodegradable in surface waters with a half-life in water on the order of days. Volatilization from water is slow. Since there is a lack of substantive data on these removal rates, we give no recommended value.

Recommended half-lives (in days):

Air 1.2 days

Soil no recommended value

Water no recommended value

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Chloroform

Other names: Trichloromethane

CAS Registry Number: 67-66-3

Chloroform is released to air and water from its many uses as a solvent, bleaching agent, and intermediate chemical in manufacturing and consumer uses. Chloroform is used as a solvent for fats, oils, rubber, alkaloids, and waxes. It is used in the manufacture of fluorocarbon refrigerants and propellants and plastics. Also in manufacturing it is a primary source for chlorodifluoromethane. It has been used as an anesthetic and in the manufacture of anesthetics and pharmaceuticals. Chloroform is also used as a fumigant, sweetener, and fire extinguisher. It is released to air from paper mills where it is used in the bleaching process. Chloroform is also an unavoidable by-product of the chlorination of water containing organic materials and is thus found in many water supplies throughout the U.S.

Formula: CCl_3H

Molecular weight

119.39 (Howard et al., 1990; Windholz et al., 1983)

119.38 (Weast et al., 1986; Verschueren, 1983)

Melting Point

-64 °C (Verschueren, 1983)

-63.5 °C (Howard et al., 1990; Windholz et al., 1983)

Octanol-water partition coefficient (K_{ow})

93.3 corresponding to a log K_{ow} of 1.97 reported by Hansch and Leo (1987) and by Leo et al. (1971) based on a value published in Hansch and Anderson (1967). This value is cited in Verschueren (1983) and in Howard et al. (1990).

- 87.1 corresponding to a log K_{ow} of 1.94 reported by Hansch and Leo (1987) based on a value published by Schauman (1938). This value was also reported by Hansch and Leo (1987) as obtained from unpublished measurements by Hansch and his colleagues.
- 79.4 measured by Banerjee et al. (1980) who report the standard deviation of the measurement error as $\pm 0.9\%$ (which corresponds to an absolute error of ± 0.7). This measurement is also cited by Hansch and Leo (1987) as a log K_{ow} of 1.90.

Recommended value, based on the log-mean value of the 3 measured values reported above:

$$\log K_{ow} = 1.94 \pm 0.035$$

$$K_{ow} = 87 \times \text{or} + 1.1$$

Vapor pressure at standard temperatures

The Merck Index (Windholz et al., 1983) reports the boiling point of chloroform as 59 °C

Stull (1947) reports the following vapor pressures (VPs) for chloroform.

Temperature (C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
0.5	60	8.0
10.4	100	13
25.9	200	26
42.7	400	53
61.3	760	101

Interpolating from this data gives VP at 25 °C = 25.9 kPa

Verschueren (1983) reports the following vapor pressures for chloroform.

Temperature (C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
20	160	21
30	245	33
62	760	101

Interpolating from this data give VP at 25 °C = 26.5 kPa

The following Antoine equations have been published for estimating the vapor pressure of chloroform in kPa

$$\log_{10}(\text{VP}) = 6.079 - \frac{1171}{226.2 + T} \quad \text{for } -10^\circ\text{C} < T < 60^\circ\text{C} \text{ from Boublik et al. (1984)}$$

which gives VP = 26.1 kPa at 25° C, and

$$\log_{10}(\text{VP}) = 5.618 - \frac{929.44}{196.03 + T} \quad \text{for } -35^\circ\text{C} < T < 61^\circ\text{C} \text{ from Dean (1985)}$$

which gives VP = 25.9 kPa at 25° C.

The Antoine equation above proposed by Boublik et al. (1984) for VP versus temperature is plotted below.

Recommended value for the temperature range -10 to 60 °C, based on the Antoine equation of Boublik et al. (1984) above:

$$VP(kPa) = 10^{[6.079 - 1171/(226.2 + T)]} \pm 0.40 \text{ for } -10 < T < 60$$

$$VP(kPa) = 26 \pm 0.4 @ 25 \text{ } ^\circ\text{C}$$

Solubility in water

- 10,000 mg/L at 15 °C reported by Verschueren (1983)
- 8000 mg/L at 20 °C reported by Verschueren (1983)
- 9300 mg/L at 15 °C reported by Verschueren (1983)
- 7400 mg/L at 25 °C reported by *The Merck Index* (Windholz et al., 1983)
- 7950 mg/L at 25 °C reported by Howard et al. (1990), who attribute this value to Mackay et al. (1980).
- 15,000 mg/L at 0 °C reported as ppm by volume by Andelman (1978). [As cited in Horvath (1982)].
- 9870 mg/L at 0 °C reported by Chancel and Parmentier (1885a,b). [As cited in Horvath (1982)].
- 9800 mg/L at 0 °C reported as wt % by Reinders and de Minjer (1947). [As cited in Horvath (1982)].
- 11,000 mg/L at 0 °C reported by Rex (1906). [As cited in Horvath (1982)].
- 9800 mg/L at 0 °C reported as mole fraction by Staverman (1941). [As cited in Horvath (1982)].
- 9800 mg/L at 0 °C reported as wt % by Washburn (1928). [As cited in Horvath (1982)].
- 10,000 mg/L at 1.5 °C reported as ppm by wt. by Dilling (1977). [As cited in Horvath (1982)].
- 8900 mg/L at 3.2 °C reported by Chancel and Parmentier (1885a,b). [As cited in Horvath (1982)].
- 13,000 mg/L at 10 °C reported as ppm by volume by Andelman (1978). [As cited in Horvath (1982)].
- 8850 mg/L at 10 °C reported as volume fraction by Larson et al. (1962) citing Ostwald (1894). [As cited in Horvath (1982)].
- 8950 mg/L at 10 °C reported by Rex (1906). [As cited in Horvath (1982)].

- 8600 mg/L at 10 °C reported as wt % by Washburn (1928). [As cited in Horvath (1982)].
- 10,000 mg/L at 15 °C reported as wt % by Antropov et al. (1972). [As cited in Horvath (1982)].
- 8400 mg/L at 15 °C reported as wt % by Evans (1936). [As cited in Horvath (1982)].
- 8500 mg/L at 15 °C reported by Gross and Saylor (1931). [As cited in Horvath (1982)].
- 10,000 mg/L at 15 °C reported as wt % by Gunther et al. (1968). [As cited in Horvath (1982)].
- 8600 mg/L at 15 °C reported as wt % by Jones et al. (1957). [As cited in Horvath (1982)].
- 10,000 mg/L at 15 °C reported as g/cc by Patty (1962). [As cited in Horvath (1982)].
- 10,000 mg/L at 15 °C reported as g/cc by Schefflan and Jacobs (1953). [As cited in Horvath (1982)].
- 8400 mg/L at 15 °C reported as wt % by Stephen and Stephen (1963). [As cited in Horvath (1982)].
- 4820 mg/L at 15 °C reported as g/g at 1 atm. pressure by Svetlanov et al. (1971). [As cited in Horvath (1982)].
- 7100 mg/L at 17.4 °C reported by Chancel and Parmentier (1885a,b). [As cited in Horvath (1982)].
- 12,000 mg/L at 20 °C reported in ppm by volume by Andelman (1978). [As cited in Horvath (1982)].
- 7900 mg/L at 20 °C reported in wt % by Antonov (1907). [As cited in Horvath (1982)].
- 8200 mg/L at 20 °C reported in wt % by du Pont (1966). [As cited in Horvath (1982)].
- 8000 mg/L at 20 °C reported in wt % by Evans (1936). [As cited in Horvath (1982)].
- 8150 mg/L at 20 °C reported in wt % by Interdyne, Inc. (1976). [As cited in Horvath (1982)].
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- 8200 mg/L at 20 °C reported in ppm by wt by Pearson and McConnell (1975). [As cited in Horvath (1982)].
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- 8200 mg/L at 20 °C reported in wt % by Riddick and Bunger (1970). [As cited in Horvath (1982)].
- 7500 mg/L at 20 °C reported by Salkowski (1920). [As cited in Horvath (1982)].
- 8200 mg/L at 20 °C reported by Schefflan and Jacobs (1953). [As cited in Horvath (1982)].
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- 8200 mg/L at 20 °C reported in ppm by wt by Selenka and Bauer (1978). [As cited in Horvath (1982)].
- 8000 mg/L at 20 °C reported by Smith (1932). [As cited in Horvath (1982)].
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- 8000 mg/L at 20 °C reported in wt % by Stephen and Stephen (1963). [As cited in Horvath (1982)].
- 8000 mg/L at 20 °C reported in wt % by Washburn (1928). [As cited in Horvath (1982)].
- 11,400 mg/L at 20 °C reported in cc/cc H₂O by Ostwald (1894) according to Larson et al. (1962). [As cited in Horvath (1982)].
- 8100 mg/L at 20 °C reported in g/g by Kirk-Othmer (1964). [As cited in Horvath (1982)].

- 7950 mg/L at 25 °C reported by Afghan and Mackay (1980). [As cited in Horvath (1982)].
- 11,500 mg/L at 25 °C reported in ppm by volume by Andelman (1978). [As cited in Horvath (1982)].
- 13,000 mg/L at 25 °C reported by Aref'eva et al. (1979). [As cited in Horvath (1982)].
- 7220 mg/L at 25 °C reported in mol/L by Banerjee et al. (1980). [As cited in Horvath (1982)].
- 13,000 mg/L at 25 °C reported in cc/100 cc water by Booth and Everson (1948). [As cited in Horvath (1982)].
- 7950 mg/L at 25 °C reported in ppm by wt by Chiou et al. (1977). [As cited in Horvath (1982)].
- 7500 mg/L at 25 °C reported in wt % by Conti et al. (1960). [As cited in Horvath (1982)].
- 7500 mg/L at 25 °C reported in ppm by wt by Dilling (1977). [As cited in Horvath (1982)].
- 8000 mg/L at 25 °C reported in wt % by Gladis (1960). [As cited in Horvath (1982)].
- 8300 mg/L at 25 °C reported in cc/g water by Lax (1967). [As cited in Horvath (1982)].
- 7900 mg/L at 25 °C reported in g/g w McGovern (1943). [As cited in Horvath (1982)].
- 7920 mg/L at 25 °C reported in wt % by Miller (1969). [As cited in Horvath (1982)].
- 8200 mg/L at 25 °C reported in wt % by Mitchell and Smith (1977). [As cited in Horvath (1982)].
- 9000 mg/L at 25 °C reported in wt % by Reinders and de Minjer (1947). [As cited in Horvath (1982)].
- 8000 mg/L at 25 °C reported in g/125 cc water by Wright and Schaffer (1932). [As cited in Horvath (1982)].
- 7050 mg/L at 29.4 °C reported by Chancel and Parmentier (1885a,b). [As cited in Horvath (1982)].
- 11,200 mg/L at 30 °C reported in ppm by volume by Andelman (1978). [As cited in Horvath (1982)].
- 7700 mg/L at 30 °C reported in wt % by Evans (1936). [As cited in Horvath (1982)].

- 7710 mg/L at 30 °C reported in g/g by Gross and Saylor (1931). [As cited in Horvath (1982)].
- 6200 mg/L at 30 °C reported in cc/cc-water by Larson et al. (1962) citing Ostwald (1894). [As cited in Horvath (1982)].
- 7760 mg/L at 30 °C reported by Rex (1906). [As cited in Horvath (1982)].
- 7700 mg/L at 30 °C reported in mole fraction by Staverman (1941). [As cited in Horvath (1982)].
- 7600 mg/L at 30 °C reported in wt % fraction by Stephen and Stephen (1963). [As cited in Horvath (1982)].
- 3200 mg/L at 30 °C reported in g/g-water at 1 atm. pressure by Svetlanov et al. (1971). [As cited in Horvath (1982)].
- 3200 mg/L at 30 °C reported in g/g-water at 1 atm. pressure by Svetlanov et al. (1971). [As cited in Horvath (1982)].
- 8200 mg/L at 30 °C reported by Svetlanov et al. (1971). [As cited in Horvath (1982)].
- 7700 mg/L at 30 °C reported in mol/100-g-H₂O by Van Arkel (1946). [As cited in Horvath (1982)].
- 7700 mg/L at 30 °C reported in mol/100-g-water by Van Arkel and Vles (1936). [As cited in Horvath (1982)].
- 7600 mg/L at 30 °C reported in wt % by Washburn (1928). [As cited in Horvath (1982)].
- 5920 mg/L at 37 °C reported in cc/cc-water by Allott et al. (1973), Steward et al. (1973–1974), Larson et al. (1962), and Papper and Kitz (1963), all citing Ostwald (1894). [As cited in Horvath (1982)].
- 6000 mg/L at 37 °C reported in cc/cc-water by Macintosh et al. (1963). [As cited in Horvath (1982)].
- 5600 mg/L at 38 °C reported in cc/cc-water by Grant (1978) citing Ostwald (1894). [As cited in Horvath (1982)].
- 6800 mg/L at 40 °C reported in cc/cc-water by Larson et al. (1962) citing Ostwald (1894). [As cited in Horvath (1982)].
- 7350 mg/L at 40 °C reported in wt % by Washburn (1928). [As cited in Horvath (1982)].
- 7120 mg/L at 41.6 °C reported by Chancel and Parmentier (1885a,b). [As cited in Horvath (1982)].
- 7100 mg/L at 42 °C reported in wt % by Reinders and de Minjer (1947). [As cited in Horvath (1982)].

- 2050 mg/L at 45 °C reported in g/g-water at 1 atm. pressure by Svetlanov et al. (1971). [As cited in Horvath (1982)].
- 7450 mg/L at 50 °C reported in wt % by Washburn (1928). [As cited in Horvath (1982)].
- 7750 mg/L at 54.9 °C reported by Chancel and Parmentier (1885a,b). [As cited in Horvath (1982)].
- 7700 mg/L at 55 °C reported in wt % by Washburn (1928). [As cited in Horvath (1982)].
- 8000 mg/L at 56.1 °C reported in wt % by Conti et al. (1960). [As cited in Horvath (1982)].
- 7500 mg/L at 60 °C reported in wt % by Reinders and de Minjer (1947). [As cited in Horvath (1982)].
- 1300 mg/L at 45 °C reported in g/g-water at 1 atm. pressure by Svetlanov et al. (1971). [As cited in Horvath (1982)].

From the information above, Horvath (1982) has constructed the following polynomial fit for the dependence of chloroform solubility (in wt %) on temperature (T) in °C in the range 0 to 60 °C

$$WS(\text{wt } \%) = 0.995 - 1.0531 \times 10^{-2} T + 7.9819 \times 10^{-5} T^2 + 6.6431 \times 10^{-7} T^3 \pm 0.001$$

which gives

$$\begin{aligned} WS &= 0.792 \pm 0.001 (\text{wt } \%) \text{ at } 25 \text{ }^\circ\text{C} \\ &= 7920 \pm 10 \text{ mg/L at } 25 \text{ }^\circ\text{C} \\ &= 66.3 \pm 0.1 \text{ mol/m}^3 \text{ at } 25 \text{ }^\circ\text{C} \end{aligned}$$

The dependence of chloroform solubility in water on temperature as given by this formula is plotted below.

Recommended value of solubility versus temperature, T in °C, based on the analysis by Horvath (1982):

$$\begin{aligned} WS(\text{mg/L}) &= 9950 - 105.31 T + 0.79819 T^2 + 0.0066431 T^3 \\ &\pm 10 \text{ mg/L for } 0 \text{ }^\circ\text{C} < T < 60 \text{ }^\circ\text{C} \end{aligned}$$

$$WS(\text{mg/L}) = 7920 \pm 10 \text{ mg/L @ } 25 \text{ }^\circ\text{C}$$

$$WS(\text{mol/m}^3) = 66.3 \pm 0.1 \text{ mol/m}^3 \text{ @ } 25 \text{ }^\circ\text{C}$$

Henry's law constant (dimensionless form)

- 0.18 at 25 °C reported by Howard et al. (1990), who attribute this value to Hine and Mookerjee (1975).
- 0.18 at 25 °C reported as the experimental value of H/RT by Hine and Mookerjee (1975).
- 0.12 at 20 °C reported by Mackay and Shiu (1981), who attribute this value to McConnell et al. (1975).
- 0.13 at 25 °C reported by Mackay and Shiu (1981), who attribute this value to Dilling (1977).
- 0.0645 at 9.6 °C with a CV of 0.062 reported by Gossett (1987).
- 0.103 at 17.5 °C with a CV of 0.020 reported by Gossett (1987).
- 0.150 at 24.8 °C with a CV of 0.038 reported by Gossett (1987).
- 0.223 at 34.6 °C with a CV of 0.020 reported by Gossett (1987).

Gossett (1987) has developed the following regression of Henry's law constant in $\text{m}^3/(\text{atm}\cdot\text{mol})$ versus temperature in K, which applies in the temperature range 10 to 35 °C

$$H = \exp(9.843 - 4612/T) \pm 4\%$$

This can be converted to the dimensionless form to give

$$H/RT = (1/T) \times \exp(19.25 - 4612/T) \pm 4\%$$

Plotted below is the dimensionless Henry's law constant H/RT versus temperature as derived from Gossett's regression above and as derived from the ratio of $VP/(WS-RT)$ using the temperature-dependent expressions for VP and WS presented above.

Recommended value of H/RT versus temperature, T in $^{\circ}\text{C}$:

$$H/RT = (1/T) \times \exp(19.25 - 4612/T) \pm 4\%$$

$$H/RT = 0.15 \pm 0.006 @ 25^{\circ}\text{C}$$

Organic-carbon partition coefficient (K_{oc})

Howard et al. (1990) report a K_{oc} of 34 measured for chloroform in two soils. Estimation methods for K_{oc} produce the following values for K_{oc} ,

- 271 as derived from the K_{oc} estimation method based on K_{ow} proposed by Kenaga and Goring (1980) and referred to in Lyman et al. (1990).
- 77.1, 65.5, 37.4, and 42.0 as derived from the four regression equations relating K_{oc} to K_{ow} in Karickhoff (1985).
- 39 as derived from the regression of K_{oc} with solubility proposed by Chiou et al. (1977)
- 31.3 as derived from the regression of K_{oc} with solubility proposed by Kenaga (1980)
- 34.5 as derived from the regression of K_{oc} with the molecular connectivity index ($^1\chi = 1.73$) as proposed by Meylan et al. (1992).

Recommended value base on the log mean of the measured and predicted values above:

$$\log K_{oc} = 1.7 \pm 0.3$$

$$K_{oc} = 53 \times \text{or} \div 2$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}} .$$

The molecular weight, M_y , of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). With the molecular volume V_x of chloroform equal to 81 cm^3/mol , this expression gives

Recommended value:

$$D_{\text{water}} = 3.6 \times 10^{-7} T \text{ m}^2/\text{d} = 1.1 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.2 \times 10^{-9} \text{ m}^2/\text{s} @ 25^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2} .$$

With the molecular volume, V_x , of chloroform of $81 \text{ cm}^3/\text{mol}$ and a molecular weight of 119.4 g/mol , the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 3.6 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.77 \text{ m}^2/\text{d} \text{ or } 8.9 \times 10^{-6} \text{ m}^2/\text{s} @ 25^\circ\text{C}$$

Steady-state bioconcentration factors for plant tissue concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for chloroform in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, $K_{\text{ps}}^{\text{rain}}$ is equal to $0.0034 \text{ kg}(\text{soil})/\text{kg}(\text{plant})$ with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, $\text{mg}/\text{kg}[\text{fresh mass}]$, to contaminant concentration in soil solution, mg/L) for chloroform as

$$\text{RCF} = 1.8$$

When this factor is divided by the sorption coefficient, $K_D = f_{oc} \times K_{oc} = (0.01 \text{ to } 0.02) \times K_{oc}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg(fresh mass) to contaminant concentration in soil solids, mg/kg, which we refer to as $K_{ps}(\text{roots})$ and estimate it as being in the range

$$K_{ps}(\text{roots}) = 0.3 \text{ to } 6$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

$$K_{ps}(\text{roots}) = 20 \text{ to } 80 \text{ (recommended range for root crops)}$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 2.8 \times \text{or} + 5.3 \text{ (recommended value for exposed produce)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for chloroform in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 0.009 \text{ m}^3/\text{kg}$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

6 reported for bluegill sunfish by Barrows et al. (1980) and cited in Howard et al. (1990).

3.34 to 10.35 reported for rainbow trout by Anderson and Lusty (1980) and cited in Howard et al. (1990).

- 1.6 to 2.5 reported for bluegill by Anderson and Lusty (1980) and cited in Howard et al. (1990).
- 2.9 to 3.1 reported for largemouth bass by Anderson and Lusty (1980) and cited in Howard et al. (1990).
- 3.3 to 3.7 reported for catfish by Anderson and Lusty (1980) and cited in Howard et al. (1990).
- 4.2 Based the K_{ow} value and the correlation of Mackay (1982).

Recommended value, based on the mean value of the range of measured values and the predicted value reported above:

$$BCF(\text{fish}) = 4 \pm 2.5$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for chloroform are available in the current literature.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for chloroform as

$$B_k = 7 \times 10^{-7} \times \text{or} \pm 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for chloroform are available in the current literature.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for chloroform as

$$B_t = 2 \times 10^{-6} \times \text{or} \pm 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for chloroform are available in the current literature.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for chloroform as

$$B_e = 7 \times 10^{-4} \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Howard et al. (1991) have estimated the half-life of chloroform in soil due to aerobic biodegradation to be in the range of four weeks to six months.

Recommended values, based on range of the soil half lives:

$$\text{aerobic soil biodegradation rate constant} = 0.0143 \text{ d}^{-1} \times \text{or} + 1.7$$

Media-specific half lives for air, soil, and surface water

- Air.* Howard et al. (1991) estimate the half life of chloroform in lower atmosphere is in the range of 623 to 6230 hours (26 to 260 days) based on photo-oxidation as a removal process.
- Soil* Howard et al. (1991) have estimated the half-live of chloroform in soil due to aqueous aerobic biodegradation to be in the range of 672 to 4320 hours (28 to 180 days).
- Water* Howard et al. (1991) have estimated the half-live of chloroform in surface water due to aqueous aerobic biodegradation to be in the range of 672 to 4320 hours (28 to 180 days).

Recommended half lives (in days), based on arithmetic mean of the half lives and geometric range of the values:

$$\text{Air} \quad 80 \times \text{or} + 1.9$$

$$\text{Soil} \quad 70 \times \text{or} + 1.7$$

$$\text{Water} \quad 70 \times \text{or} + 1.7$$

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Di-2-Ethylhexylphthalate (DEHP)

Other names: di-octylphthalate (DOP), bis-(2-ethylhexyl) phthalate, 1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester, Octoil

CAS Registry Number: 117-81-7

Di-2-ethylhexylphthalate is used in large quantities in the organic chemical industry primarily as a plasticizer for polyvinyl chloride and other polymeric materials (Howard, 1989). It is also used as organic pump fluid. DEHP is released to air and water during the production, disposal, incineration, and recycling of plastic materials in which it has been used.

Formula: $C_{24}H_{38}O_4$

Molecular weight

390.54 (Howard, 1989; Windholz et al., 1983)

Melting Point

10 °C (Verschueren, 1983)

11.8 °C (Howard, 1989)

Octanol-water partition coefficient (K_{ow})

9,550 based on a log K_{ow} of 3.98 reported by Hansch and Leo (1987) and referenced to a value published by Scheele (1980). However, in the Scheele (1980) paper, which lists this value, no statement is made as to whether this is a measured, estimated, or cited value.

45,700 based on a log K_{ow} of 4.66 reported by Harnisch et al. (1983) as a measured value from the OECD/EEC laboratory comparison tests for the shake-flask method.

- 87,100 based on a log K_{ow} of 4.94 reported by Harnisch et al. (1983) as a measured value from the OECD/EEC laboratory comparison tests for the shake-flask method.
- 89,100 based on a log K_{ow} of 4.95 reported by Harnisch et al. (1983) as a measured value from the OECD/EEC laboratory comparison tests for the shake-flask method.
- 151,000 based on a log K_{ow} of 5.18 reported by Harnisch et al. (1983) as a measured value from the OECD/EEC laboratory comparison tests for the shake-flask method.
- 107,000 based on a log K_{ow} of 5.03 reported by Hansch and Leo (1987) and referenced to the measured values published in Harnisch et al. (1983)
- 129,000 based on a log K_{ow} of 5.11 as given in Howard (1989) and attributed to Howard et al (1985)
- 275,000 based on a log K_{ow} of 5.44 reported by Harnisch et al. (1983) as a measured value from the OECD/EEC laboratory comparison tests for the shake-flask method.
- 8.7×10^7 Based on a log K_{ow} value of 7.94 as measured in Howard et al. (1985). However, Howard et al (1985) report that this value is suspect because the method they used may not work well with this compound. [This value is also cited in Hansch and Leo (1987).

Recommended value, based on the log-mean value of the 6 measured values reported above but excluding the suspect value reported by Howard et al. (1983):

$$\log K_{ow} = 5.05 \pm 0.26$$

$$K_{ow} = 112,000 \times \text{or} \div 1.8$$

Vapor pressure at standard temperatures

- 0.00034 Pa at 25 °C measured using the gas saturation method by Howard et al. (1985).
- 0.00064 Pa at 25 °C measured using the gas saturation method by Howard et al. (1985).
- 0.00083 Pa at 25 °C measured by Werner (1952).
- 0.00086 Pa at 25 °C reported by Howard (1989) based on the mean of the values measured by Howard et al. (1985).

0.0016 Pa at 25 °C measured using the gas saturation method by Howard et al. (1985).

670 Pa at 230 °C reported by Howard (1989).

160 Pa at 200 °C reported by Verschueren (1983).

From the measured vapor pressures reported above, the following approximate Antoine equation can be developed:

$$\log_{10} (\text{VP in Pa}) = 11.297 - \frac{4281.3}{273 + T}, \text{ which gives VP} = 0.0085 \text{ Pa at } 25^\circ \text{ C.}$$

The Antoine equation proposed above for VP versus temperature is plotted below in the temperature range $-10^\circ \text{C} < T < 40^\circ \text{C}$.

Recommended value based on the mean of the 4 measured values cited above:

$$\text{VP(Pa)} = 0.00085 \pm 0.0005 \text{ Pa @ } 25^\circ \text{ C}$$

Solubility in water

0.041 mg/L at 20 °C measured by Leyder and Boulenger (1983). [This value is also cited in Howard et al. (1985)].

- 0.285 mg/L at 24 °C for technical grade DEHP reported by Verschueren (1983).
 0.34 ± 0.04 mg/L at 25 °C measured by Howard et al. (1985). [This value is also cited in Howard (1989)].
 0.40 ± 0.05 mg/L at 25 °C measured by Wolf et al. (1980a). [This value is also cited in Howard et al. (1985)].

Recommended water solubility (WS) based on the arithmetic mean of all the reported values above:

$$WS(\text{mg/L}) = 0.27 \pm 0.16 \text{ mg/L @ } 25 \text{ }^{\circ}\text{C}$$

$$WS(\text{mol/m}^3) = 6.9 (\pm 4.1) \times 10^{-4} \text{ mol/m}^3 \text{ @ } 25 \text{ }^{\circ}\text{C}$$

Henry's law constant (dimensionless form, i.e., H/RT)

- 4.5 × 10⁻⁴ at 25 °C calculated by Howard (1989) based on the ratio of vapor pressure to solubility.
 4.9 (± 4.1) × 10⁻⁴ at 25 °C derived from the mean and standard deviation of the ratio vapor pressure and solubility based on the values reported in sections above.

Recommended value, based on the values reported above:

$$H/(RT) = 4.9 (\pm 4.1) \times 10^{-4} \text{ @ } 25 \text{ }^{\circ}\text{C}$$

Organic-carbon partition coefficient (K_{oc})

- 5,800 calculated by Kenaga (1980).
 57,000 calculated by Wolfe et al. (1980b)
 87,420 reported by Russell and McDuffie (1986) in a 1.59% organic-carbon composite soil from Broome County, New York. [Also cited in Howard, 1989)]
 1400 ± 200 based on measurements by Sullivan et al. (1982) of DEHP desorption from ocean sediment samples containing roughly 1% organic carbon.
 With K_{ow} = 112,000 (log K_{ow} = 5.05) and WS = 0.27 mg/L, estimation methods for K_{oc} produce the following values for K_{oc},

- 13,300 as derived from the regression equation relating K_{oc} to K_{ow} in Kenaga and Goring (1980) and referred to in Lyman et al. (1990).
- 13,400; 104,000; 44,500; and 54,100 as derived from the four regression equations relating K_{oc} to K_{ow} in Karickhoff (1985).
- 23,000 as derived from the regression of K_{oc} with water solubility proposed by Chiou et al. (1977)
- 8,970 as derived from the regression of K_{oc} with water solubility proposed by Kenaga (1980)
- 166,000 calculated by Meylan et al (1992) with a regression equation relating K_{oc} to the molecular connectivity index ($^1\chi = 13.6$).

Recommended value, based on the log-mean value of the 12 values reported above and the 68% (2 GSD) range about the log mean:

$$\log K_{oc} = 4.3 \pm 0.67$$

$$K_{oc} = 20,000 \times \text{or} \div 4.7$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}}$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume, V_x , estimated by the LeBas incremental method, described in Lyman et al. (1990) equals $459 \text{ cm}^3/\text{mol}$. With these values and with temperature (T) expressed in kelvins, this expression gives,

Recommended value:

$$D_{\text{water}} = 1.3 \times 10^{-7} T \text{ m}^2/\text{d} = 3.8 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 4.3 \times 10^{-10} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller, et al. (1966) method described in Lyman et al. (1982), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of DEHP of $459 \text{ cm}^3/\text{mol}$ and a molecular weight of 391 g/mol , and with temperature (T) expressed in kelvins, this expression gives

Recommended value:

$$D_{\text{air}} = 1.5 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.33 \text{ m}^2/\text{d} \text{ or } 3.8 \times 10^{-6} \text{ m}^2/\text{s} @ 25^\circ \text{C}$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for DEHP in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash,

$K_{\text{ps}}^{\text{rain}}$ is equal to $0.0034 \text{ kg(soil)/kg(plant)}$ with a CV of 1 (Dreicer et al. 1984).

This partition factor relates plant fresh-mass concentration to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, $\text{mg/kg}[\text{fresh mass}]$, to contaminant concentration in soil solution, mg/L) for DEHP as

$$\text{RCF} = 0.82 + 0.03 K_{\text{ow}}^{0.77} = 233$$

When this factor is divided by the sorption coefficient, $K_D = f_{\text{oc}} \times K_{\text{oc}} = (0.01 \text{ to } 0.02) \times K_{\text{oc}}$ (from above), we obtain the ratio of contaminant concentration in roots, $\text{mg/kg}(\text{fresh mass})$ to contaminant concentration in soil solids, mg/kg , which we refer to as $K_{\text{ps}}(\text{roots})$ and estimate it as being in the range

$$K_{\text{ps}}(\text{roots}) = 0.46 \text{ to } 0.93 \times \text{or} \div 4.4 \text{ (reflecting the estimation error in } K_{\text{oc}})$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

(recommended value for root crops)

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 1.2 \times \text{or} + 4.4 \quad (\text{reflecting the error in } K_{oc})$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 0.02 \times \text{or} + 5.4 \quad (\text{recommended value for exposed produce reflecting the estimation error in the regression equation})$$

Bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for DEHP in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 2300 \quad (\text{recommended value})$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1 (or GSD = 2.3).

Bioconcentration factors for fish concentration relative to water or sediment concentrations

209 ± 65 measured by Brown and Thompson (1982a) in *Daphnia magna* (waterfleas).

2370 to 2630 measured by Brown and Thompson (1982b) in *Mytilus edulis* (mussels).

13500 to 13600 measured by Sanders et al. (1973) at 25 °C in Scud.

- 260 to 270 measured by Sanders et al. (1973) at 25 °C in Scud.
- 5200 measured by Sanders et al. (1973) at 25 °C in Waterfleas.
- 3100 measured by Sanders et al. (1973) at 25 °C in Midge larvae.
- 129 peak value measured in fish by Metcalf et al. (1973) in a study to determine uptake of 10 ppm DEHP in water by aquatic organisms.
- 265 peak value measured in fish by Metcalf et al. (1973) in a study to determine uptake of 0.1 ppm DEHP in water by aquatic organisms.
- 155 peak value measured in waterfleas by Metcalf et al. (1973) in a study to determine uptake of 10 ppm DEHP in water by aquatic organisms.
- 183 peak value measured in waterfleas by Metcalf et al. (1973) in a study to determine uptake of 0.1 ppm DEHP in water by aquatic organisms.
- 402 peak value measured in snails by Metcalf et al. (1973) in a study to determine uptake of 10 ppm DEHP in water by aquatic organisms.
- 858 peak value measured in snails by Metcalf et al. (1973) in a study to determine uptake of 0.1 ppm DEHP in water by aquatic organisms.
- 420 measured in waterfleas after 7 days exposure by Mayer and Sanders (1973) using a water concentration of 0.3 µg/L.
- 3600 measured in scud after 14 days exposure by Mayer and Sanders (1973) using a water concentration of 0.1 µg/L.
- 350 measured in midges after 7 days exposure by Mayer and Sanders (1973) using a water concentration of 0.3 µg/L.
- 1380 measured in flathead minnows after 28 days exposure by Mayer and Sanders (1973) using a water concentration of 1.9 µg/L.
- 247 based on measurements of DEHP concentration in rainbow trout bile relative to that in water by Statham et al. (1976).

Recommended value, based on the log-mean value of the 16 values reported above and the 68% (2 GSD) range about the log mean:

$$\log \text{BCF} = 2.86 \pm 0.63$$

$$\text{BCF} = 720 \times \text{ or } \div 4.3$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for DEHP are available in the current literature. An estimation method for this parameter is considered below.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for DEHP as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 8.9 \times 10^{-4} \times \text{or} + 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for DEHP are available in the current literature. An estimation method for this parameter is considered below.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for DEHP as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 2.8 \times 10^{-3} \times \text{or} + 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for DEHP are available in the current literature. An estimation method for this parameter is considered below.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for DEHP as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 0.89 \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Based on screening biodegradation studies, DEHP degrades rapidly in the presence of water, DEHP degrades rapidly in acclimated systems, but acclimation is very important since almost no degradation occurs in unacclimated systems (Howard et al., 1991). Based on grab-sample die-away test data from Schouten et al. (1979) and Johnson and Lulves (1975), Howard et al. (1991) have estimated the half-life of DEHP in soil due to aerobic biodegradation to be in the range of 5 to 23 days. Howard et al. (1991) have estimated the half-life of DEHP in soil due to anaerobic biodegradation to be in the range of 42 to 389 days. These estimates of soil biodegradation are based on unacclimated aqueous biodegradation.

Recommended value, based on log mean and log variance of the range of the soil half lives given above:

$$\text{Soil biodegradation rate constant} = 0.016 \text{ d}^{-1} \times \text{or} \pm 3.5$$

Media-specific half lives for air, soil, and surface water

- Air.* Based on measurements of dimethyl phthalate photolysis by Atkinson (1987), Howard et al. (1991) estimate that the half life of DEHP in the lower atmosphere is in the range of 2.9 to 29 hours (0.12 to 1.2 days) as a result primarily of photo-oxidation as a removal process.
- Soil* Howard et al. (1991) have estimated the half-live of DEHP in soil due to aqueous aerobic biodegradation to be in the range of 5 to 23 days. Howard et al. (1991) have estimated the half-live of DEHP in soil due to aqueous anaerobic biodegradation to be in the range of 42 to 389.
- Water* Howard et al. (1991) have estimated the half-live of DEHP in surface water due to aqueous aerobic biodegradation to be in the range of 5 to 23 days.

Recommended half-lives (in days), based on the log mean of the half lives and geometric range of the values:

Air $0.38 \times \text{or} \pm 1.9$

Soil $44 \times \text{or} \pm 3.5$

Water $11 \times \text{or} \pm 1.5$

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1,4-Dioxane

Other names: glycoethylenether; 1,4-diethylenedioxide

CAS Registry Number: 123-91-1

1,4-dioxane is a widely used solvent in chemical manufacturing. It is miscible in water and relatively soluble in organic liquids. 1,4-Dioxane is produced in millions of kg per year (Howard, 1990). It is widely used as a solvent in such commonly used products as paints, varnishes, lacquers, cosmetics, and deodorants. It is also used as a solvent for varnish removers, for wetting and dispersing agents in textile manufacturing, for dye baths, for stain and printing compositions, for cleaning and detergent preparations, and for cements. It is used as a stabilizer for chlorinated solvents and is used in scintillation fluids. 1,4-Dioxane is also used as a solvent for cellulose acetate, ethyl cellulose, benzyl cellulose, resins, oils, waxes, oil and spirit-soluble dyes.

Formula: C₄ H₈ O₂

Molecular weight

88.10 (Howard, 1990; Windholz et al., 1983)

88.11 (Weast et al., 1986)

88.20 (Verschueren, 1983)

Melting Point

10 °C (Verschueren, 1983)

11.8 °C (Howard et al., 1990)

Octanol-water partition coefficient (K_{ow})

0.537 based on a log K_{ow} of -0.27 reported by Hansch and Leo (1987) based on an unpublished analysis by P. Jow and C. Hansch.

0.537 based on a log K_{ow} of -0.27 reported by Howard et al. (1990) and referenced to a value published in Hansch and Leo (1985).

0.380 based on a log K_{ow} of -0.42 reported by Verschueren (1983) and attributed to Leo and Hansch (1971).

0.380 based on a log K_{ow} of -0.42 reported in Hansch and Leo (1987) and attributed to a measured value by Collander (1951).

Recommended value, based on the log-mean value and range of the 2 measured values reported above:

$$\log K_{ow} = -0.345 \pm 0.043$$

$$K_{ow} = 0.45 \times \text{or} \div 1.1$$

Vapor pressure at standard temperatures

Stull (1947) reports the following vapor pressures for 1,4-dioxane.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
-12.8	5	0.667
-1.2	10	1.33
12.0	20	2.67
25.2	40	5.33
33.8	60	8.00
45.1	100	13.3
62.3	200	26.7
81.8	400	53.3
101.1	760	101

Interpolating from this data set gives VP at 25 °C = 5.32 kPa

Verschueren (1983) reports the following vapor pressures for 1,4 dioxane.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
20	30	4.00
25	37	4.93
30	50	6.67
101	760	101

Interpolating from this data set give VP at 25 °C = 5.10 kPa

The Merck Index (Windholz et al., 1983) reports the following vapor pressures for 1,4-dioxane, which appear to be taken from Stull (1947).

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
12.0	20	2.67
25.2	40	5.33
33.8	60	8.00
45.1	100	13.3
62.3	200	26.7
81.8	400	53.3
101.1	760	101

5.07 kPa at 25 °C reported by Howard (1990), who attribute this value to Boublik et al (1984).

The following Antoine equations have been published for estimating the vapor pressure of 1,4-dioxane in kPa

$$\log_{10}(\text{VP}) = 6.56014 - \frac{1556.98}{240.566 + T} \text{ for } 20\text{ }^{\circ}\text{C} < T < 105\text{ }^{\circ}\text{C} \text{ from Boublik et al. (1984),}$$

which gives VP = 4.98 kPa at 25° C;

$$\log_{10}(\text{VP}) = 6.56891 - \frac{1558.445}{240.459 + T} \text{ for } 20\text{ }^{\circ}\text{C} < T < 125\text{ }^{\circ}\text{C} \text{ from Boublik et al. (1984),}$$

which gives VP = 4.99 kPa at 25° C; and

$$\log_{10}(\text{VP}) = 6.5565 - \frac{1554.68}{240.34 + T} \text{ for } 20\text{ }^{\circ}\text{C} < T < 105\text{ }^{\circ}\text{C} \text{ from Dean (1985),}$$

which gives VP = 4.98 kPa at 25° C.

In addition, we have determined that a fit to the data of Stull (1947) can be obtained from the following Antoine equation

$$\log_{10}(\text{VP}) = 6.9948 - \frac{1868.13}{273 + T} \text{ for } -13\text{ }^{\circ}\text{C} < T < 45\text{ }^{\circ}\text{C} ,$$

which gives VP = 5.32 kPa at 25° C.

The Antoine equation above and the Antoine equation proposed by Boublik et al. (1984) based on the range $20\text{ }^{\circ}\text{C} < T < 105\text{ }^{\circ}\text{C}$ are both plotted in the figure above for VP versus temperature for $-10\text{ }^{\circ}\text{C} < T < 410\text{ }^{\circ}\text{C}$ and compared to measured values by Stull (1947).

Recommended value of vapor pressure for the temperature range -10 to $40\text{ }^{\circ}\text{C}$, based on the Antoine equation proposed here:

$$\text{VP(kPa)} = 10^{[6.9948 - 1868.13/(273 + T)]} \times \text{or} \div 1.02 \text{ for } -10\text{ }^{\circ}\text{C} < T < 40\text{ }^{\circ}\text{C}$$

Recommended value at $25\text{ }^{\circ}\text{C}$, based on the range of values above:

$$\text{VP(kPa)} = 5.12 \pm 0.15 @ 25\text{ }^{\circ}\text{C}$$

Solubility in water

1,4-dioxane is miscible with water, which means that any amount of 1,4-dioxane and water will combine in solution.

Henry's law constant (dimensionless form, i.e. H/RT)

- 2.0×10^{-4} based on the measured infinite dilution activity coefficient, f_{∞} of 5.6 at 25 °C by Cabani et al. (1971) and the vapor pressure, VP, reported above, 5120 Pa. The activity coefficient is used to find C_a/C_w according to $C_a/C_w = f_{\infty} (VP/RT) \times 10^{-6} \text{ m}^3/\text{g}(\text{water}) \times 18 \text{ g/mol}(\text{water})$].
- 2.0×10^{-4} at 25 °C reported by Hine and Mookerjee (1975) who attribute this value to Cabani et al. (1971). The value is also cited in Howard (1989), who attributes it to Hine and Mookerjee (1975)].
- 3.7×10^{-4} at 25 °C measured by Amoores and Buttery (1979).

Recommended value, based on the log-mean value and range of the 2 measured values reported above:

$$H/(RT) = 2.8 (\pm 0.50) \times 10^{-4} \text{ @ } 25 \text{ }^{\circ}\text{C}$$

Organic-carbon partition coefficient (K_{oc})

No reported measurements of K_{oc} or K_d for 1,4-dioxane in soils or sediments are available in the current literature. With $K_{ow} = 0.45$ ($\log K_{ow} = -0.345$) estimation methods for K_{oc} produce the following values for K_{oc} ,

- 15 as derived from the regression equation relating K_{oc} to K_{ow} in Kenaga and Goring (1980) and referred to in Lyman et al. (1990).
- 1.7, 0.29, 0.21, and 0.22 as derived from the four regression equations relating K_{oc} to K_{ow} in Karickhoff (1985).
- 4.1 as derived from the regression as proposed by Meylan et al (1992) of K_{oc} with the molecular connectivity index ($^1\chi = 3.0$) and a correction factor of -2.528 for the two aliphatic-ether C-O bonds.

Recommended value, based on the log-mean value of the 6 values reported above and the 68% 2 GSD range about the log mean:

$$\log K_{oc} = 0.56 \pm 0.73$$

$$K_{oc} = 3.7 \times \text{ or } \div 5.4$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}} .$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With the molecular volume V_x 1,4-dioxane equal to 84 cm^3/mol , this expression gives

Recommended value:

$$D_{\text{water}} = 3.5 \times 10^{-7} T \text{ m}^2/\text{d} = 1.0 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.2 \times 10^{-9} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1982), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of 1,4-dioxane equal to 84 cm^3/mol and a molecular weight of 88.1 g/mol, the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 3.7 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.79 \text{ m}^2/\text{d} \text{ or } 9.1 \times 10^{-6} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for 1,4-dioxane in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} is equal to 0.0034 kg(soil)/kg(plant) with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, mg/kg[*fresh mass*], to contaminant concentration in soil solution, mg/L) for 1,4-dioxane as

$$RCF = 0.82 + 0.03 K_{ow}^{0.77} = 0.84$$

When this factor is divided by the sorption coefficient, $K_d = f_{oc} \times K_{oc} = (0.01 \text{ to } 0.02) \times K_{oc}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg(*fresh mass*) to contaminant concentration in soil solids, mg/kg, which we refer to as $K_{ps}(\text{roots})$ and estimate it as being in the range

$$K_{ps}(\text{roots}) = 11 \text{ to } 23 \times \text{or} + 5.4 \text{ (reflecting the estimation error in } K_{oc})$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain:

Recommended value for root crops,

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 280 \times \text{or} + 5.4 \text{ (reflecting the error in } K_{oc})$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient:

Recommended value for exposed produce,

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 12 \times \text{or} + 5.4 \text{ (reflecting the estimation error in the regression).}$$

Bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for 1,4-dioxane in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{m^3}{kg} = 1.4$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1 (or GSD = 2.3).

Bioconcentration factors for fish concentration relative to water or sediment concentrations

No information on the bioconcentration factor for 1,4-dioxane could be found in the literature. However, based on its K_{ow} value, its estimated bioconcentration factor is 0.02 based on the correlation of Mackay (1982). However, since this is significantly less than 1 and we do not expect fish to have significantly lower levels of 1,4-dioxane than the water surrounding them, it seems reasonable to assume a BCF on the order of 1.

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for 1,4-dioxane are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for 1,4-dioxane as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 3.6 \times 10^{-9} \times \text{or} \div 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for 1,4-dioxane are available in the current literature. Estimation methods for this parameter are considered below.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for 1,4-dioxane as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 1.1 \times 10^{-8} \times \text{or} \div 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for 1,4-dioxane are available in the current literature. An estimation method value for this parameter is considered below.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed in Part I, we estimate the egg biotransfer factor for 1,4-dioxane as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 3.6 \times 10^{-6} \times \text{or} \div 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Kawasaki (1980) reports that, because of the presence of oxygen in cyclic form, 1,4-dioxane is resistant to biodegradation. Howard et al. (1991) have estimated the half-life of 1,4-dioxane in soil due to aerobic biodegradation to be in the range of no less than one month to an estimated high value of 6 months. Howard et al. (1991) have estimated the half-life of 1,4-dioxane in soil due to anaerobic biodegradation to be in the range of no less than 4 months to an estimated high value of 24 months. These estimates of soil biodegradation are based on unacclimated aqueous biodegradation.

Recommended value, based on log mean and log variance of the range of the soil half lives given above:

$$\text{Soil biodegradation rate constant} = 0.005 \text{ d}^{-1} \times \text{or} \div 2.5$$

Media-specific half lives for air, soil, and surface water

- Air.** 1,4-dioxane is not directly degraded by photolysis in air Howard et al. (1991). Based on measurements by Atkinson (1987), Howard et al. (1991) estimate the half life of 1,4-dioxane in lower atmosphere is in the range of 8.1 to 81 hours (0.34 to 3.4 days) based on photo-oxidation as a removal process.
- Soil** Howard et al. (1991) have estimated the half-live of 1,4-dioxane in soil due to aqueous aerobic biodegradation to be in the range of 672 to 4320 hours (28 to 180 days). Howard et al. (1991) have estimated the half-live of 1,4-dioxane in soil due to aqueous anaerobic biodegradation to be in the range of 2688 to 17280 hours (112 to 720 days).
- Water** Howard et al. (1991) have estimated the half-live of 1,4-dioxane in surface water due to aqueous aerobic biodegradation to be in the range of 672 to 4320 hours (28 to 180 days).

Recommended half-lives (in days), based on the log mean of the half lives and geometric range of the values:

Air $1.9 \times \text{or} + 1.9$

Soil $142 \times \text{or} + 2.5$

Water $71 \times \text{or} + 1.7$

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Hexachlorobenzene

Other names: HCB, perchlorobenzene, Anticarie, Bunt-cure, Bunt-no-more, Julin's carbon chloride

CAS Registry Number: 118-74-1

Hexachlorobenzene (HCB) is formed as a waste product in the production of several chlorinated hydrocarbons and is a contaminant in some pesticides. HCB is released to air as a fugitive emission from hydrocarbon production facilities and is also released to air in flue gases and fly ash from waste incineration. HCB is persistent in the environment due to its chemical stability and resistance to biodegradation. (Howard, 1989).

Formula: C_6Cl_6

Molecular weight

284.78 (Weast et al., 1986)

284.79 (Mackay et al., 1992)

284.8 (Howard, 1989; Verschueren, 1983; Windholz et al., 1983)

Octanol-water partition coefficient (K_{ow})

1.35×10^4 derived from a log K_{ow} of 4.13 reported by Hansch and Leo (1985) based on the value measured by Lu and Metcalf (1975). [Also cited in Mackay et al. (1992)].

- 1.00×10⁵ derived from a log K_{ow} of 5.00 reported by Hansch and Leo (1985) based on the value measured by Könemann et al. (1979). [Also cited in Mackay et al. (1992)].
- 1.70×10⁵ derived from a log K_{ow} of 5.23 reported by Mackay et al. (1992) based on the value measured by Veith et al. (1979).
- 2.51×10⁵ derived from a log K_{ow} of 5.40 reported by Hansch and Leo (1985) based on the value measured by Wateral et al. (1982). [Also cited in Mackay et al. (1992)].
- 2.95×10⁵ derived from a log K_{ow} of 5.47 reported by Mackay et al. (1992) based on the value measured by Sarna et al. (1984).
- 2.95×10⁵ derived from a log K_{ow} of 5.47 reported by Hansch and Leo (1985) based on the value measured by Miller et al. (1984). [Also cited in Mackay et al. (1992)].
- 3.16×10⁵ derived from a log K_{ow} of 5.5 reported by Mackay et al. (1992) based on the value measured by Pereira et al. (1988).
- 3.16×10⁵ derived from a log K_{ow} of 5.50 reported by Mackay et al. (1992) based on the value measured by Chiou et al. (1982).
- 4.0×10⁵ derived from a log K_{ow} of 5.6 reported by Mackay et al. (1992) based on the value measured by Brooke et al. (1986).
- 4.37×10⁵ derived from a log K_{ow} of 5.64 reported by Mackay et al. (1992) based on the value measured by Mailhot (1987).
- 4.57×10⁵ derived from a log K_{ow} of 5.66 reported by Hansch and Leo (1985) based on the value measured by Hammers et al. (1982). [Also cited in Mackay et al. (1992)].
- 4.57×10⁵ derived from a log K_{ow} of 5.66 reported by Mackay et al. (1992) based on the value measured using shake-flask and gas chromatography by Eadsforth and Moser (1983).
- 5.37×10⁵ derived from a log K_{ow} of 5.73 reported by Mackay et al. (1992) based on the value measured by De Bruijn et al. (1989).
- 3.16×10⁵ derived from a log K_{ow} of 5.75 reported by Mackay et al. (1992) based on the value measured by Garst and Wilson (1984).
- 7.9×10⁵ derived from a log K_{ow} of 5.9 reported by Mackay et al. (1992) based on the value measured by Brooke et al. (1986).
- 1.66×10⁶ derived from a log K_{ow} of 6.22 reported by Mackay et al. (1992) based on the value measured by McDuffie (1981).

- 1.66×10⁶ derived from a log K_{ow} of 6.22 reported by Mackay et al. (1992) based on the value measured by Doucette and Andren (1988).
- 1.86×10⁶ derived from a log K_{ow} of 6.27 reported by Hansch and Leo (1985) based on the value measured by Könemann et al. (1979). [Also cited in Mackay et al. (1992)].
- 2.39×10⁶ derived from a log K_{ow} of 6.38 reported by Mackay et al. (1992) based on the value measured using high pressure liquid chromatography by Eadsforth and Moser (1983).
- 8.32×10⁶ derived from a log K_{ow} of 6.92 reported by Mackay et al. (1992) based on the value measured by De Kock and Lord (1987).

Recommended value, based on the log-mean value of the 20 measured values reported above:

$$\log K_{ow} = 5.68 \pm 0.58$$

$$K_{ow} = 4.79 \times 10^5 \times \text{or} \div 3.8$$

Vapor pressure in Pa at standard temperatures

- 0.00028 reported at 25 °C by Sears and Hopke (1949). [Also cited in Mackay et al. (1992)].
- 0.00145 reported at 20 °C by Kilzer et al (1979). [Also cited in Mackay et al. (1992)].
- 0.0023 reported at 25 °C by Farmer et al (1980). [Also cited in Mackay et al. (1992)].
- 0.000453 reported at 25 °C by Klein et al. (1981). [Also cited in Mackay et al. (1992)].
- 0.000167 reported at 25 °C by Klein et al. (1981). [Also cited in Mackay et al. (1992)].
- 0.00046 reported at 25 °C by Dobbs and Cull (1982). [Also cited in Mackay et al. (1992)].
- 0.0006 reported at 20 °C by Gükel et al. (1982). [Also cited in Mackay et al. (1992)].
- 0.303, 0.159, 0.121 values quoted and measured for subcooled liquid at 25 °C by Bidleman (1984). [Also cited in Mackay et al. (1992)].

Gükel et al. (1982) have developed an Antoine equation relating vapor pressure to temperature (T in °C) for hexachlorobenzene in the temperature range 20 to 60 °C,

$$\log \text{VP}(\text{torr}) = 12.37 - 5152.1/(273 + T) \text{ or}$$

$$\log \text{VP}(\text{Pa}) = 14.49 - 5152.1/(273 + T)$$

This equation gives VP = 0.0016 at 25 °C

Recommended value for the temperature range 20 to 60 °C, based on the Antoine equation above and adjusted to give the log mean value of the measured values reported above:

$$\log \text{VP} = 14.1 - 5152.1/(273 + T) \pm 0.40$$

$$\text{VP} = 0.00065 \times \text{ or } + 2.5 @ 25 \text{ °C}$$

The adjusted Antoine equation above for VP versus temperature is plotted below.

Solubility in water

- 0.006 mg/L [no temperature specified] (Verschueren, 1983).
- 0.004 mg/L [no temperature specified] (Verschueren, 1983).
- 0.0062 mg/L at 25 °C reported by Howard (1989), who attributes this value to Farmer et al. (1977).
- 0.005 mg/L at 25 °C reported by Weil et al. (1974). [Also cited in Horvath (1982) and Mackay et al. (1992)].
- 0.006 mg/L at 25 °C reported by Lu and Metcalf (1975). [Also cited in Horvath (1982) and Mackay et al. (1992)].
- 0.10 mg/L at 24 °C reported by Hollifield (1979). [Also cited in Horvath (1982) and Mackay et al. (1992)].
- 0.005 mg/L at 25 °C reported by Yalkowsky et al. (1979). [Also cited in Horvath (1982) and Mackay et al. (1992)].
- 0.0039 mg/L at 25 °C reported by Könemann (1981). [Also cited in Mackay et al. (1992)].
- 0.0054 mg/L at 25 °C reported by Hashimoto et al. (1982). [Also cited in Mackay et al. (1992)].
- 0.0012 to 0.014 (0.004 geometric mean) mg/L at 25 °C reported by Hashimoto et al. (1982). [Also cited in Mackay et al. (1992)].
- 0.0047 mg/L at 25 °C reported by Miller et al. (1984). [Also cited in Mackay et al. (1992)].

Recommended value based on the arithmetic mean of the measured values above excluding the value reported by Hollifield (1979):

$$WS = 0.005 \pm 0.0007 \text{ mg/L @ } 25 \text{ }^{\circ}\text{C}$$

$$1.7 \times 10^{-5} \pm 2 \times 10^{-6} \text{ mol/m}^3 \text{ @ } 25 \text{ }^{\circ}\text{C}$$

Henry's law constant (dimensionless form, i.e. H/RT)

- 0.028 reported at 20 °C by Callahan et al. (1979). [Also cited in Mackay et al. (1992)].
- 0.053 reported at 25 °C by Atlas et al. (1982) based on batch stripping. [Also cited in Mackay et al. (1992)].

0.020 reported at 25 °C by Oliver and Niimi (1985) based on batch stripping. [Also cited in Mackay et al. (1992)].

0.054 reported at 25 °C by Nirmalakhandan and Speece (1988). [Also cited in Mackay et al. (1992)].

Recommended value based on the arithmetic mean of the measured values above:

$$H/RT = 0.04 \pm 0.015 @ 25 ^\circ\text{C}$$

The figure below is the plot of the dimensionless Henry's law constant based on the ratio of temperature-dependent vapor pressure to solubility as recommended in sections above

Dimensionless Henry's law versus temperature for HCB

Organic-carbon partition coefficient (K_{oc})

- 3.63×10² derived from a log K_{oc} of 2.56 measured (using Speyer soil < 200 mm particle diameter) by Rippen et al. (1982) [Also cited in Mackay et al. (1992)].
- 5.01×10² derived from a log K_{oc} of 2.70 measured (using Alfisol) by Rippen et al. (1982) [Also cited in Mackay et al. (1992)].
- 3.89×10³ derived from a log K_{oc} of 3.59 measured by Kenaga (1980) and also reported in Kenaga and Goring (1980) [Also cited in Mackay et al. (1992)].
- 2.81×10⁴ derived from a log K_{oc} of 4.45 reported by Kenaga (1980) [Also cited in Mackay et al. (1992)].
- 5.89×10⁴ derived from a log K_{oc} of 4.77 from the value measured by Hodson and Williams (1988) [Also cited in Mackay et al. (1992)].
- 7.94×10⁴ derived from a log K_{oc} of 4.90 from measured values from bottom sediment by Karickhoff and Morris (1985) [Also cited in Mackay et al. (1992)].
- 7.94×10⁵ derived from a log K_{oc} of 5.90 from measured field data by Oliver and Charlton (1984) [Also cited in Mackay et al. (1992)].
- 7.94×10⁵ derived from a log K_{oc} of 5.90 from measured field data by Oliver and Charlton (1984) [Also cited in Mackay et al. (1992)].
- 1.26×10⁶ derived from a log K_{oc} of 6.1 from measured suspended sediments in the Great Lakes watershed by Oliver (1987a) [Also cited in Mackay et al. (1992)].
- 2.00×10⁶ derived from a log K_{oc} of 6.3 from the mean of the Niagara River plume measurements by Oliver (1987b) [Also cited in Mackay et al. (1992)].

Recommended value, based on the log-mean value of the 10 measured values reported above:

$$\log K_{oc} = 4.7 \pm 1.4$$

$$K_{oc} = 5.0 \times 10^4 \times \text{or} + 25$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}}$$

The molecular weight, M_y , of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With the molecular volume V_x of HCB equal to 221 cm^3/mol , this expression gives

Recommended value:

$$D_{\text{water}} = 2.0 \times 10^{-7} T \text{ m}^2/\text{d} = 5.8 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 6.7 \times 10^{-10} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller, et al. (1966) method described in Lyman et al. (1982), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of HCB of 221 cm^3/mol and a molecular weight of 285 g/mol, the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 2.2 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.47 \text{ m}^2/\text{d} \text{ or } 5.4 \times 10^{-6} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Bioconcentration factors for plant tissue concentration relative to soil concentration

- 0.0034 mg/kg(fresh plant) per mg/kg(fresh soil) is the partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.
- 0.25 ± 0.094 mg/kg(fresh plant) per mg/kg(fresh soil) based on a partition factor of 0.90 ± 0.34 as measured by Beall (1976) between grass and soil in the 0 to 2 cm depth on a dry-soil and dry-grass basis. We assume that the ratio of plant dry mass to fresh mass is on the order of 0.25 and that the ratio of soil dry mass to soil fresh mass is on the order of 0.9.
- 0.42 ± 0.18 mg/kg(fresh plant) per mg/kg(fresh soil) based on a partition factor of 1.49 ± 0.63 as measured by Beall (1976) between grass and soil in the 0 to 4 cm depth on a dry-soil and dry-grass basis. We assume that the ratio of plant dry mass to fresh mass is on the order of 0.25 and that the ratio of soil dry mass to soil fresh mass is on the order of 0.9.
- 0.55 ± 0.41 mg/kg(fresh plant) per mg/kg(fresh soil) as measured by Dejonckheere et al. (1975) of HCB residues in lettuce and in soil taken from 0 to 20 cm depth.
- 0.13 mg/kg(fresh plant) per mg/kg(fresh soil) based on a partition factor of 0.48 mg/kg(dry plant) per mg/kg(dry soil) reported by Travis and Arms (1988) and attributed to Beall (1976) and Dejonckheere et al. (1975). We assume that the ratio of plant dry mass to fresh mass is on the order of 0.25 and that the ratio of soil dry mass to soil fresh mass is on the order of 0.9.

Recommended value based on the three the measured values reported above excluding the rainsplash factor:

$$K_{ps} = 0.41 \pm 0.26 \text{ mg/kg(fresh plant) per mg/kg(fresh soil)}$$

Bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for HCB in air are available in the current literature. An estimation methods for this parameter is thus applied

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{m^3}{kg} = 190$$

We assume the CV associated with it is on the order of 1.

Recommended value:

$$K_{pa}^{gs} = 190 \times \text{or} \div 2.2$$

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

- 1.2×10^3 derived from a fish/water log BCF of 3.09 reported by Körte et al. (1978) [Also cited in Mackay et al. (1992)].
- 1.9×10^4 derived from a flathead-minnow/water log BCF of 4.27 reported by Veith et al. (1979b). [Also cited in Mackay et al. (1992)].
- 5.4×10^3 derived from a rainbow-trout/water log BCF of 3.73 reported by Veith et al. (1979b). [Also cited in Mackay et al. (1992)].
- 2.2×10^4 derived from a green sunfish/water log BCF of 4.34 reported by Veith et al. (1979b). [Also cited in Mackay et al. (1992)].
- 2.9×10^5 derived from a guppy-lipid/water log BCF of 5.46 reported by Könnemann and van Leeuwen (1980). [Also cited in Mackay et al. (1992)].
- 1.9×10^4 derived from a fish/water log BCF of 4.27 reported by Ciam et al. (1980). [Also cited in Mackay et al. (1992)].
- 8.5×10^3 derived from a fish/flowing-water log BCF of 3.93 reported by Kenaga and Goring (1980). [Also cited in Mackay et al. (1992)].
- 2.9×10^2 derived from a fish/static-water log BCF of 2.46 reported by Kenaga and Goring (1980). [Also cited in Mackay et al. (1992)].
- 1.5×10^4 derived from a rainbow-trout/water log BCF in the range 4.08 to 4.3 (mean 4.19) reported by Oliver and Niimi (1983). [Also cited in Mackay et al. (1992)].

- 1.9×10^5 derived from a rainbow-trout-lipid/water log BCF in the range 5.16 to 5.37 (mean 5.27) reported by Oliver and Niimi (1983). [Also cited in Mackay et al. (1992)]. {Based on values above, this implies a fish-lipid content of 8 %.}
- 2.3×10^3 derived from a fish/water log BCF of 3.36 reported by Klein et al. (1984). [Also cited in Mackay et al. (1992)].
- 2.6×10^3 derived from a fish/water log BCF of 3.41 reported by Freitag et al. (1984). [Also cited in Mackay et al. (1992)].
- 2.2×10^4 derived from a flathead-minnow/water log BCF of 4.34 reported by Carlson and Kosian (1987). [Also cited in Mackay et al. (1992)].
- 2.0×10^4 derived from a fish/water log BCF of 4.3 reported by Oliver (1987c). [Also cited in Mackay et al. (1992)].
- 2.6×10^6 derived from a Atlantic-croaker-lipid/water log BCF of 6.42 reported by Pereira et al. (1988). [Also cited in Mackay et al. (1992)].
- 5.1×10^6 derived from a blue-crab-lipid/water log BCF of 6.71 reported by Pereira et al. (1988). [Also cited in Mackay et al. (1992)].
- 9.1×10^5 derived from a spotted-sea-trout-lipid/water log BCF of 5.96 reported by Pereira et al. (1988). [Also cited in Mackay et al. (1992)].
- 9.5×10^5 derived from a blue-catfish-lipid/water log BCF of 5.98 reported by Pereira et al. (1988). [Also cited in Mackay et al. (1992)].

Recommended value, based on the log-mean value of the 18 measured values reported above (lipid-based BCFs are adjusted downward by a factor of 0.08 to account for fish lipid content):

$$\log \text{BCF}(\text{fish}) = 4.2 \pm 0.8$$

$$\text{BCF}(\text{fish}) = 1.6 \times 10^4 \times \text{or} + 6.3$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

0.016 ± 0.0028 mg/kg(whole milk) per mg/d based on an biotransfer factor for dairy cows of 0.39 ± 0.070 d/kg(milk fat) as measured by Fries and Marrow (1976) between milk fat and daily uptake. We assume that whole milk is 4% fat.

0.00015 ± 0.000077 mg/kg(whole milk) per mg/d based on an milk-diet partition coefficient for dairy cows of 0.0015 ± 0.00077 as measured by Borzelleca

et al (1976) between milk and diet. We assume that the cows in this study consumed ~ 10 kg milking-chow per day.

0.0085 mg/kg(whole milk) per mg/d based on the biotransfer factor reported by Travis and Arms (1988) and attributed to Fries and Marrow (1976) and Borzelleca et al (1976).

Recommended value, based on the mean value and range of the 2 measured values reported above:

$$B_k = 0.0081 \times \text{or} \div 2.8 \text{ or}$$

$$\log B_k = -2.09 \pm 0.45$$

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

0.092 ± 0.016 mg/kg(fresh meat) per mg/d based on an biotransfer factor for body fat of cows of 0.37 ± 0.065 d/kg(body fat) as measured by Fries and Marrow (1976) between milk fat and daily uptake. We assume that fresh meat is 25 % fat.

0.0024 ± 0.00084 mg/kg(fresh meat) per mg/d based on an fat-diet bioconcentration factor [mg/kg(fat) per mg/kg(diet)] for cows of 0.076 ± 0.027 as measured by Borzelleca et al (1976). We assume that the cows in this study consumed ~ 8 kg of dry feed per day and that fresh meat is 25 % fat.

0.045 mg/kg(fresh meat) per mg/d based on the biotransfer factor reported by Travis and Arms (1988) and attributed to Fries and Marrow (1976) and Borzelleca et al (1976).

Recommended value, based on the mean value and range of the 2 measured values reported above:

$$B_t = 0.047 \times \text{or} \div 2.8 \text{ or}$$

$$\log B_t = -1.33 \pm 0.45$$

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for HCB are available in the current literature. An estimation method value for this parameter is considered below.

If we assume that the fat-diet partition factor in chickens is similar to that in cattle, then the fat-to-diet biotransfer values reported above can be used to estimate K_{fd} as 1.7 ± 2.0 mg/kg(fat) per mg/kg(diet). Then based on a fat content of eggs of 0.08 kg(fat)/kg(contents) and a feed intake of 0.12 kg(fresh mass)/d by chickens, we obtain the following estimate of a biotransfer factor, B_e , from chicken diet to eggs with units d/kg(eggs)

$$B_e = 1.1 \times \text{or} \div 8.6$$

$$\log B_e = 0.041 \pm 0.9$$

The coefficient of variation attributable to the extrapolation of fat-diet bioconcentration factors from cows to chickens is assumed to be a factor of 10.

Contaminant biodegradation factors in soil

Beck and Hansen (1974) have reported the aqueous, *aerobic* biodegradation half-life of HCB in unacclimated soil grab samples in the range 23,256 to 50,136 hours (2.7 to 5.7 years). [This study is also cited in Howard et al. (1991) and Mackay et al. (1992)]. This range of soil half-lives corresponds to a soil biodegradation rate constant of 0.12 to 0.26 yr⁻¹.

Beck and Hansen (1974) have reported the aqueous, *anaerobic* biodegradation half-life of HCB in unacclimated soil grab samples in the range 93,024 to 200,544 hours (11 to 22 years). This range of soil half-lives corresponds to a soil biodegradation rate constant of 0.032 to 0.063 yr⁻¹.

Recommended values, based on arithmetic mean of the soil half lives:

$$\text{aerobic soil biodegradation rate constant} = 0.18 \text{ y}^{-1} \times \text{or} \div 1.3$$

$$\text{anaerobic soil biodegradation rate constant} = 0.044 \text{ y}^{-1} \times \text{or} \div 1.2$$

Media-specific half lives for air, soil, and surface water

- Air.** Howard et al. (1991) estimate the half life of HCB in lower atmosphere is in the range of 3750 to 37500 hours (0.43 to 4.2 years) based on photo oxidation as a removal process.
- Soil** Howard et al. (1991) have estimated the half-live of HCB in soil due to aerobic biodegradation to be in the range of 2.7 to 5.7 years.
- Water** Howard et al. (1991) have estimated the half-live of HCB in surface water due to aerobic biodegradation to be in the range of 2.7 to 5.7 years.

Recommended values, based on arithmetic mean of the half lives and geometric range of the values:

<i>Air</i>	2.3 × or + 3 years
<i>Soil</i>	4.2 × or + 1.5 years
<i>Water</i>	4.2 × or + 1.5 years

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Inorganic Arsenic (As)

Over 100 minerals and ores contain arsenic (Bodek et al., 1988). In nature, arsenic is usually associated with sulfide ores. Arsenic has valence states of -3, 0, +3 or +5. The principal arsenic-bearing minerals include arsenopyrite (FeAsS), niccolite (NiAsS), cobaltite (CoAsS), tennantite ($\text{Cu}_{12}\text{As}_4\text{S}_{13}$), enargite (Cu_3AsS_4), and native arsenic. The principal arsenic compounds produced for industrial use are arsenic trioxide (As_2O_3) and arsenic metal. From these other arsenic compounds are made. About 70% of all arsenic consumed by industry is used in pesticides. Other uses of arsenic and arsenic compounds are in wood preservatives, glass manufacturing, alloys, electronics, catalysts, feed additives, and veterinary chemicals (Bodek et al., 1988). The forms of inorganic arsenic found in waters and soils include arsenious acids such as H_3AsO_3 , $\text{H}_2\text{AsO}_3^{-1}$, and HAsO_3^{-2} , and arsenic acids such as H_3AsO_4 , $\text{H}_2\text{AsO}_4^{-1}$, and HAsO_4^{-2} , as well as arsenite ($\text{H}_2\text{AsO}_3^{-1}$) compounds, arsenate ($\text{H}_2\text{AsO}_4^{-1}$) compounds, and arsine gas (AsH_3). Arsine is only produced in extremely anoxic environments and appears to be rapidly oxidized under aerobic conditions or in the atmosphere.

Molecular and atomic weights

- 74.92 g/mol, atomic weight of As (Bowen, 1979; Weast et al., 1986).
- 77.93 g/mol, molecular weight of arsine gas, AsH_3 (Windholz et al., 1983).
- 141.93 g/mol, molecular weight of arsenic acid, H_3AsO_4 (Windholz et al., 1983).
- 197.84 g/mol, molecular weight of arsenic trioxide, As_2O_3 (Weast et al., 1986).
- 386.72 g/mol, molecular weight of arsenic pentoxide, As_2O_5 (Weast et al., 1986).

Melting points

- 814 °C for arsenic metal, As [but only at high pressure ~28 atm., at atmospheric pressure it boils before melting (Stull, 1947).
- 312.8 °C for arsenic trioxide, As_2O_3 (Stull, 1947).
- 35.5 °C for arsenic acid, H_3AsO_4 (Weast et al., 1986).
- 116.3 °C for arsine gas, AsH_3 (Stull, 1947).

Vapor pressure

- 610 °C is the boiling point of arsenic, As (Stull, 1947).
- 160 °C is the boiling point of arsenic acid, H_3AsO_4 (Weast et al., 1986).
- 457.2 °C is the boiling point of arsenic trioxide, As_2O_3 (Stull, 1947).

Stull (1947) reports the following vapor pressures for arsenic trioxide (As_2O_3).

Temperature ($^{\circ}\text{C}$)	Vapor Pressure (mm)	Vapor Pressure (kPa)
212.5	1	0.133
242.6	5	0.667
259.7	10	1.33
279.2	20	2.67
299.2	40	5.33
310.3	60	8.00
332.5	100	13.3
370.0	200	26.7
412.2	400	53.3
457.2	760	101

Interpolating from this data gives VP at $25^{\circ}\text{C} = 10^{-3} \text{ Pa}$

Stull (1947) reports the following vapor pressures for arsine gas (AsH_3).

Temperature ($^{\circ}\text{C}$)	Vapor Pressure (mm)	Vapor Pressure (kPa)
-142.6	1	0.133
-130.8	5	0.667
-124.7	10	1.33
-117.7	20	2.67
-110.2	40	5.33
-104.8	60	8.00
-98.0	100	13.3
-87.2	200	26.7
-75.2	400	53.3
-62.1	760	101

Interpolating from this data gives VP at $25^{\circ}\text{C} = 7 \text{ kPa}$

Recommended value:

No recommended vapor pressure for inorganic arsenic since it is there is no significant VP for any arsenic compound other than arsine gas, which is quickly transformed in the environment.

Solubility in water

In aqueous systems, arsenic forms anions in solution, and thus it does not form complexes with simple anions such as Cl^- or SO_4^- (Bodek et al., 1988). Anionic arsenic complexes behave like ligands in water. In aerobic aqueous systems, the arsenic acids $\text{H}_2\text{AsO}_4^{-1}$ and HAsO_4^{-2} are the dominant species in the pH range 2 to 11. Below pH 2, the arsenious acid, $\text{H}_2\text{AsO}_3^{-1}$ can be the dominant species in reducing conditions and above pH 12, the arsenious acid, HAsO_3^{-2} appears.

metal arsenic, As, is insoluble in water (Weast et al., 1986).

0.2 L/L (8.0 mol/m^3 at 25°C and 1 atm. assuming an ideal gas) of arsine gas, (AsH_3) (Weast et al., 1986).

12,000 mg/L (60.65 mol/m^3) of arsenic trioxide (As_2O_3), at 5°C (Weast et al., 1986).

115,000 mg/L (580 mol/m^3) of arsenic trioxide (As_2O_3), at 100°C (Weast et al., 1986).

767,000 mg/L (1980 mol/m^3) of arsenic pentoxide (As_2O_5), at 100°C (Weast et al., 1986).

470,000 mg/L (3311 mol/m^3) of arsenic acid (H_3AsO_4) in "hot" water (Weast et al., 1986).

1,500,000 mg/L (3880 mol/m^3) of arsenic pentoxide (As_2O_5), at 16°C (Weast et al., 1986).

2,840,000 mg/L ($20,000 \text{ mol/m}^3$) of arsenic acid (H_3AsO_4) at 12.5°C (Weast et al., 1986).

<p>Recommended values for water solubility (WS):</p> <p>WS(As metal) = ~ 0</p> <p>WS(Arsine gas) = $\sim 8 \text{ mol/m}^3$ @ 25°C</p> <p>WS(As^{+3}) = 8 to 200 mol/m^3 in at ambient temperatures</p> <p>WS(As^{+5}) = 4,000 to $12,000 \text{ mol/m}^3$ in aerobic environments at ambient temperatures</p>
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Henry's law constant

0.35 estimated dimensionless Henry's law constant (H/RT) for Arsine (AsH_3) based on the vapor pressure and solubility information provided above.

Because of their almost complete speciation in water and extremely low vapor pressures, most arsenic compounds do not have measurable or predicted Henry's law constants. However, at low concentrations, the ratio of air to water concentration in air and water environments that are in contact can be estimated as

$$C_w/C_a = A \times v_d / (V_w \times R_w)$$

where C_w is the arsenic concentration in a given water body, mol/m³; C_a is the arsenic concentration in air above the water body, mol/m³; v_d is the deposition velocity that represents the rate of arsenic transfer from air to water, m/d; A is the contact area between the air and water, m²; V_w is the volume of the water body, m³; and R_w is the first-order rate constant that accounts for all arsenic removals from water (i.e. precipitation and deposition), day⁻¹.

Partition coefficients in soils and sediments

- 62 to 170 L/kg reported by Wauchope and McDowell (1984) in lake sediments for As (V) when the As concentration in water is 0.37 µmol/L. [As cited in Bodek et al. (1988).]
- 88 to 179 L/kg reported by Wauchope and McDowell (1984) in lake sediments for As (V) when the As concentration in water is 3.97 µmol/L. [As cited in Bodek et al. (1988).]
- 243 (2.3) L/kg are the mean and geometric standard deviation (in parentheses) of the distribution coefficient (K_d) reported by Sakata (1987) for As (III) in 15 different soils.
- 512 to 5500 L/kg reported by Arthur D. Little (1984) in alluvial material for total arsenic. [As cited in Bodek et al. (1988).]
- 128 to 5500 L/kg reported by Arthur D. Little (1984) in residual soil from a landfill for total arsenic. [As cited in Bodek et al. (1988).]
- 521 to 2500 L/kg reported by Arthur D. Little (1984) in silty fine sand with little clay for total arsenic. [As cited in Bodek et al. (1988).]
- 71 to 254 L/kg reported by Arthur D. Little (1984) in gravelly, well-graded silty sand for total arsenic. [As cited in Bodek et al. (1988).]
- 162 to 455 L/kg reported by Arthur D. Little (1984) in brown, clayey sand for total arsenic. [As cited in Bodek et al. (1988).]

15 to 110 L/kg reported by Arthur D. Little (1984) in fine sand for total arsenic.
[As cited in Bodek et al. (1988).]

Bodek et al. (1988) list Langmuir constants for arsenic (V). These equations give the following estimates of the distribution coefficient K_d in soils.

$$K_d = S/C = A_m K_L / (1 + K_L C) \quad [\text{L/kg}]$$

where

S is the arsenic sorbed to soil, mol/kg;

C is the arsenic concentration in soil water, mol/L;

A_m is the maximum amount of arsenic that can be absorbed by soil and ranges from 0.0072 to 0.0099 mol/kg; and

K_L is the measure of bond strength holding the sorbed arsenic to the soil surface and ranges from 3500 to 3700 L/mol.

The two solid lines in the figure below represent this range of distribution coefficients associated with the range of Langmuir constants quoted above.

Elkhatib et al. (1984) have reported values for As (III) sorption by various soils in West Virginia and fit Freundlich isotherms to model sorption for five of these soils. The following Freundlich-isotherm derived distribution coefficients, K_d , bracket the range of isotherms developed by Elkhatib et al. (1984),

$$K_d = S/C = 19.2 C^{0.958} / C \quad [\text{L/kg}]$$

$$K_d = S/C = 28.3 C^{0.399} / C \quad [\text{L/kg}]$$

where S is the sorbed arsenic (III) concentration, mg/kg, and C is arsenic (III) concentration in water, mg/L. The dashed lines in the figure below illustrate the dependence of the distribution coefficient for arsenic on arsenic concentration in the water phase based on these Freundlich isotherms.

Recommended value of K_d for arsenic in soils and in sediments based on the geometric mean and geometric standard deviation of values considered above:

$$15 \leq K_d \leq 5500$$

$$\log K_d = 2.44 \pm 0.67$$

$$K_d = 274 \times \text{or} \div 4.7$$

Diffusion coefficient in water

In dilute solutions of ionized species, such as arsenic compounds, in which there are no rapid chemical reactions and the solution is isothermal, Bodek et al. (1988) have shown that diffusion coefficients for the anions and cations in solution do not vary greatly and are on the order of $1.5 \times 10^{-9} \text{ m}^2/\text{s}$. The diffusion coefficients of many simple salts generally do not vary by more than a factor of 2 over a range of concentrations and temperatures even though their conductivities can vary greatly (Bodek et al., 1988).

Recommended value:

$$D_{\text{water}} = 1.3 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.5 \times 10^{-9} \text{ m}^2/\text{s} \times \text{or} \pm 2 \text{ for } 0^\circ\text{C} \leq T \leq 40^\circ\text{C}$$

Diffusion coefficient in air

Because of the extremely low vapor pressure of arsenic and inorganic arsenic compounds, these chemical species are not likely to be found in the gas phase of the environment. There is no need for a diffusion coefficient in air and, thus no value is recommended.

Bioconcentration factors for plant tissue concentration relative to soil concentration kg(soil)/ kg(plant fresh mass), K_{ps}

Arsenic is considered an essential trace element for plants and animals (Mertz, 1981). As a likely result of uptake in water, arsenic is absorbed by roots and readily translocated to other plant parts (Bodek et al. (1988).

0.004 to 0.012 based on a soil-to-plant-dry-mass coefficient of 0.040 used by Baes et al. (1984) for the vegetative portion of food crops and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.0006 to 0.0018 based on soil-to-plant-dry-mass coefficient of 0.006 used by Baes et al. (1984) for the non-vegetative (reproductive) portion of food crops and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.0013 to 1.4 based on a 1.5 mg/kg as geosphere average of soil arsenic concentration and 0.02 to 7 mg/kg (dry mass) as a geosphere average of land-plant arsenic concentration reported by Bowen (1979) and our assumed plant dry mass fraction in the range 0.1 to 0.3.

$0.01 \times \text{or} + 34$ based on a 2 to 200 mg/kg as the range of background soil arsenic levels and 0.1 to 10 mg/kg (dry mass) as the range of background soil plant levels reported by Bodek et al. (1988) and our assumed plant dry mass fraction in the range 0.1 to 0.3.

$0.0034 \times \text{or} + 2.2$ is the partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} (Dreicer et al. 1984).

Recommended value of K_{ps} based on the log mean of the ranges of values considered above (excluding rainsplash),

$$\log K_{ps} = -2.1 \pm 1.3$$

$$K_{ps} = 0.008 \times \text{or} + 20 \text{ kg(soil)/kg(plant fresh mass)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

According to Bodek et al. (1988), airborne deposition is believed to contribute to concentrations of arsenic found in plant leaves. At low concentrations, the ratio of plant leaf concentration to air concentration when air and plant environments are in contact, can be estimated as

$$C_p/C_a = A \times v_d / (V_p \times R_p)$$

where C_p is arsenic concentration in the plants in contact with contaminated air, mol/m³; C_a is the arsenic concentration in air above the plants, mol/m³; v_d is the deposition velocity that represents the rate of arsenic transfer from air to plant surfaces, m/d; A is the contact area between the air and plants, m²; V_p is the volume of the plants compartment, m³; and R_p is the first-order rate constant that accounts for all arsenic removals from plants (i.e. wash-off, biodegradation, etc.), day⁻¹.

Bioconcentration factors for fish relative to water or sediment concentrations

333 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater fish, freshwater invertebrates, marine invertebrates, and marine fish relative to water concentration.

11 to 540 based on 0.0037 mg/L as a geosphere average of ocean-water arsenic concentration and 0.2 to 10 mg/kg (dry mass) as an average of marine-fish arsenic concentration reported by Bowen (1979) and our assumed fish dry mass fraction in the range 0.2.

Recommended BCF value, based on the geometric mean and geometric standard deviation reflecting the range of BCF values described above:

$$\log \text{BCF}(\text{fish}) = 2.3 \pm 0.63$$

$$\text{BCF}(\text{fish}) = 200 \times \text{or} \div 4.3$$

Steady-state biotransfer factors for milk or dairy-products concentration relative to contaminant intake by cattle, B_k

Stevens (1991) evaluated several studies investigating the concentration of soluble forms of arsenic (As) in milk relative to the As intake in feed.

6.2×10^{-5} d/L is uptake to milk from feed based on radioisotope studies reported by Ng (1982).

0 to 3×10^{-4} d/L is the range of values Stevens (1991) identified in studies investigating the concentration of soluble forms of arsenic (As) in milk, relative to the As intake in feed.

3×10^{-5} d/L was derived from a study by Vreman et al. (1986) by Stevens (1991) who recommended this estimate of this biotransfer factor.

Recommended biotransfer factor, B_k , for milk based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_k = -4.4 \pm 0.83$$

$$B_k = 4 \times 10^{-4} \times \text{or} \div 6.8$$

Steady-state biotransfer factors for meat relative to contaminant intake by cattle, pigs, and chickens

Stevens (1992) evaluated several studies investigating the concentration of soluble forms of arsenic (As) in meat from cattle, relative to the As intake in feed by these cattle.

5×10^{-4} to 2.4×10^{-3} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of arsenic (As) in bovine muscle relative to the As intake in feed.

1.0×10^{-3} to 3.6×10^{-3} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of arsenic (As) in bovine kidney relative to the As intake in feed.

1.8×10^{-3} to 3.0×10^{-3} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of arsenic (As) in bovine liver relative to the As intake in feed.

1.3×10^{-3} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for arsenic to bovine muscle.

2.5×10^{-3} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for arsenic to bovine liver.

2.1×10^{-3} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for arsenic to bovine kidney.

Recommended biotransfer factor, B_t , for meat based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_t = -2.75 \pm 0.27$$

$$B_t = 0.0018 \times \text{or} + 1.9$$

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for arsenic are available in the current literature.

Ng (1982) has shown that for the seven elements strontium, rubidium, iodine, cesium, cerium, plutonium, and americium, the ratio of egg contents biotransfer to beef biotransfer is $60 \times \text{or} + 13$. Based on this observation, the meat biotransfer above can be used to make an estimate of egg contents biotransfer of $0.11 \times \text{or} + 13$.

Recommended biotransfer factor, B_e , for eggs:

$$\log B_e = -0.97 \pm 1.1$$

$$B_e = 0.11 \times \text{or} + 13$$

Contaminant biodegradation factors in soil

Although laboratory experiments have demonstrated arsenic methylation in lake sediments, there is no evidence of biodegradation of inorganic arsenic in soils (Bodek et al. 1988). Thus there is no recommended biodegradation factor for inorganic arsenic compounds in soils.

Media-specific half lives for air, soil, and surface water

There is no evidence that inorganic arsenic compounds react in air, soil, or water in such a way as to increase an existing physical removal of arsenic from these compartments. Thus the half lives of arsenic species in these compartments will depend entirely upon the removal rate due to natural physical processes such as deposition and erosion.

Recommended half-lives:

<i>Air</i>	deposition half life
<i>Soil</i>	erosion half life
<i>Water</i>	suspended particle half life

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Inorganic Lead (Pb)

Lead (Pb) is the most abundant naturally occurring heavy element, appearing primarily in the form of galena (PbS), an ore that is relatively insoluble. Lead has a valence of 2 or 4. Other forms of lead found in the environment are plattnerite (PbO₂), cerussite or lead carbonate (PbCO₃) and anglesite (PbSO₄) Bodek et al. (1988). Large quantities of lead (both as metal and as oxide) are used in storage batteries. Lead compounds have been used extensively in paints. Lead oxide (PbO) is used in producing fine "crystal glass" and "flint glass."

Molecular and atomic weights

207.2 g/mol is the crustal average atomic weight of Pb (Weast et al., 1986).

Atomic weight on earth is slightly variable due to variations in stable isotope abundance. Stable isotopes and their fractional abundances (in parentheses) are: ²⁰⁴Pb (0.0148), ²⁰⁶Pb (0.236), ²⁰⁷Pb (0.226), and ²⁰⁸Pb (0.523) (Bowen, 1979). Natural isotopes of lead include ²¹⁰Pb (21 y half life), ²¹⁴Pb (26.8 m half life), which are part of the uranium decay series; ²¹²Pb (10.6 h half life), which is part in the thorium decay series; and ²¹¹Pb (36 m half life), which is part of the uranium decay series.

267.21 g/mol, molecular weight of lead carbonate, PbCO₃ (Weast et al., 1986).

223.20 g/mol, molecular weight of lead oxide, PbO (Weast et al., 1986).

239.20 g/mol, molecular weight of lead dioxide, PbO₂ (Weast et al., 1986).

303.26 g/mol, molecular weight of lead sulfate, PbSO₄ (Weast et al., 1986).

239.26 g/mol, molecular weight of lead sulfide, PbS (Weast et al., 1986).

Melting points

327.5 °C for lead metal, Pb (Stull, 1947).

1114 °C for lead sulfide, PbS (Stull, 1947).

890 °C for lead oxide, PbO (Stull, 1947).

Vapor pressure

Stull (1947) reports the following vapor pressures for lead sulfide (PbS).

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
852	1	0.133
928	5	0.667
975	10	1.33
1005	20	2.67
1048	40	5.33
1074	60	8.00
1108	100	13.3
1160	200	26.7
1221	400	53.3
1281	760	101

Interpolating from this data with an Antoine-type equation gives

VP at 25 °C = 10^{-27} Pa

Recommended value:

No recommended vapor pressure because it is virtually impossible to measure for Pb at environmental temperatures.

Solubility in water

The free hydrated Pb^{+2} is predominant in freshwater systems in the pH range typical of natural environments (Bodek et al. 1988). However, PbHCO_3^{+1} , PbCO_3 , and PbOH^{+1} can also be present in freshwater. PbCl^{+1} is the dominant species in seawater for normal pH ranges, but Pb^{+2} , PbCl_2 , and PbCl_3^{-1} are also found in seawater in the normal pH range (Bodek et al. 1988).

metal lead, Pb, is only soluble in strong acids (Weast et al., 1986).

lead dioxide, PbO_2 , is insoluble in water at ambient temperatures and pH, (Weast et al., 1986).

Pb^{+2} solubility increases with decreasing pH.

1.1 mg/L (0.0041 mol/m^3) of lead carbonate, PbCO_3 , at 20 °C (CRC, 1986).

- 17 mg/L (0.076 mol/m³) of lead oxide, PbO, at 20 °C (Weast et al., 1986).
 42.5 mg/L (0.14 mol/m³) of lead sulfate, PbSO₄, at 25 °C ((Weast et al., 1986).
 56 mg/L (0.18 mol/m³) of lead sulfate, PbSO₄, at 40 °C (Weast et al., 1986).
 0.86 mg/L (0.0036 mol/m³) of lead sulfide, PbS, at 13 °C (Weast et al., 1986).

Recommended value:

$$WS(Pb) = \sim 0$$

Depending on the availability of S, SO₄, and CO₃ anions, the pH and temperature in the water phase, the solubility of the Pb⁺² ion can vary significantly. However, for soils and surface waters with a relatively high oxygen and CO₃ anion and other ligands levels,

$$WS(Pb^{+2}) = 0.01 \text{ to } 0.1 \text{ mol/m}^3$$

Henry's law constant

Because of their almost complete speciation in water and extremely low vapor pressures, lead compounds do not have measurable or predicted Henry's law constants. However, at low concentrations, the ratio of air to water concentration in air and water environments that are in contact can be estimated as

$$C_w/C_a = A \times v_d / (V_w \times R_w)$$

where C_w is the total lead concentration in a given water body, mol/m³; C_a is the lead concentration in air above the water body, mol/m³; v_d is the deposition velocity that represents the rate of Pb transfer from air to water, m/d; A is the contact area between the air and water, m²; V_w is the volume of the water body, m³; and R_w is the first-order rate constant that accounts for all Pb removals from water (i.e. precipitation and deposition), day⁻¹.

Partition coefficients in soils and sediments

Bodek et al. (1988) list Langmuir constants for lead in various soils at pH 7.0. The resulting Langmuir equations give estimates of the distribution coefficient K_d in soils and sediments according to the following,

$$K_d = S/C = A_m K_L / (1 + K_L C) \quad [\text{L/kg}]$$

where

S is the lead sorbed to soil, mol/kg;

C is the lead concentration in soil water, mol/L;

A_m is the maximum amount of lead that can be absorbed by soil and ranges from 0.007 to 0.031 mol/kg; and

K_L is the measure of bond strength holding the sorbed lead to the soil surface and ranges from 5000 to 79,000 L/mol.

The higher of these ranges is described by Bodek et al (1988) as being more typical of sediments.

The two solid lines in the figure below represent the range of distribution coefficients associated with the range of Langmuir constants quoted above.

Bodek et al. (1988) recommend the following Freundlich-isotherm derived distribution coefficients, K_d ,

$$K_d = S/C = 2200 C^{0.926}/C \quad [\text{L/kg}] \text{ for sediments}$$

$$K_d = S/C = 15000 C^{0.2}/C \quad [\text{L/kg}] \text{ for sediments}$$

where S is the sorbed lead concentration, $\mu\text{mol/kg}$, and C is lead concentration in water, $\mu\text{mol/L}$. The dashed lines in the figure below illustrate the dependence of the distribution coefficient for lead on lead concentration in the water phase based on these Freundlich isotherms.

Recommended value of K_d for lead in soils and in sediments based on the range of values considered above:

$$20 \leq K_d \leq 5000$$

$$\log K_d = 2.5 \pm 0.69$$

$$K_d = 320 \times \text{or} + 5$$

Diffusion coefficient in water

In dilute solutions of ionized species, such as lead compounds, in which there are no rapid chemical reactions and the solution is isothermal, Bodek et al. (1988) have shown that diffusion coefficients for the anions and cations in solution do not vary greatly and are on the order of $1.5 \times 10^{-9} \text{ m}^2/\text{s}$. The diffusion coefficients of many simple salts generally do not vary by more than a factor of 2 over a range of concentrations and temperatures even though their conductivities can vary greatly (Bodek et al., 1988).

Recommended value:

$$D_{\text{water}} = 1.3 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.5 \times 10^{-9} \text{ m}^2/\text{s} \times \text{or} + 2 \text{ for } 0^\circ\text{C} \leq T \leq 40^\circ\text{C}$$

Diffusion coefficient in air

Because of the extremely low vapor pressure of lead and inorganic lead compounds, these chemical species are not likely to be found in the gas phase of the environment. There is no need for a diffusion coefficient in air and, thus, no value is recommended.

Bioconcentration factors for plant tissue concentration relative to soil concentration kg(soil)/ kg(plant fresh mass), K_{ps}

Lead is considered a non-essential element for plants. As a likely result of passive uptake in water, lead is absorbed by roots and concentrated there with little translocation to other plant parts (Bodek et al. (1988).

0.0045 to 0.0135 based on a soil-to-plant-dry-mass coefficient of 0.045 used by Baes et al. (1984) for the vegetative portion of food crops and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.0009 to 0.003 based on a soil-to-plant-dry-mass coefficient of 0.009 used by Baes et al. (1984) for the non-vegetative (reproductive) portion of food crops and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.003 to 0.1 based on a 35 mg/kg as geosphere average of soil lead concentration and 1 to 13 mg/kg (dry mass) as a geosphere average of land-plant lead concentration reported by Bowen (1979) and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.0006 to 0.2 based on a 35 mg/kg as geosphere average of soil lead concentration and 0.2 to 20 mg/kg (dry mass) as a geosphere average of edible-vegetable lead concentration reported by Bowen (1979) and our assumed plant dry mass fraction in the range 0.1 to 0.3.

$0.009 \times \text{or} + 16$ based on a 2 to 200 mg/kg as the range of background soil lead levels and 0.1 to 10 mg/kg (dry mass) as the range of background soil plant levels reported by Bodek et al. (1988) and our assumed plant dry mass fraction in the range 0.1 to 0.3.

0.0003 to 0.073 is the range of lead plant-to-soil concentration factors (on a plant fresh-mass basis reported by Ng (1982).

$0.0034 \times \text{or} + 2.3$ is the partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} (Dreicer et al., 1984).

Recommended value of K_{ps} based on the log mean of the ranges of values considered above (excluding rainsplash),

$$\log K_{ps} = -2.2 \pm 0.98$$

$$K_{ps} = 0.006 \times \text{or} + 9.5 \text{ kg(soil)/kg(plant fresh mass)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

According to Bodek et al. (1988), airborne deposition is believed to contribute to concentrations of lead found in plant leaves. At low concentrations, the ratio of plant leaf concentration to air concentration when air and plant environments are in contact, can be estimated as

$$C_p/C_a = A \times v_d / (V_p \times R_p)$$

where C_p is lead concentration in the plants in contact with contaminated air, mol/m³; C_a is the lead concentration in air above the plants, mol/m³; v_d is the deposition velocity that represents the rate of lead transfer from air to plant surfaces, m/d; A is the contact area between the air and plants, m²; V_p is the volume of the plants compartment, m³; and R_p is the first-order rate constant that accounts for all lead removals from plants (i.e. wash-off, biodegradation, etc.), day⁻¹.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

Although lead is a nonessential element, marine fish have been shown to accumulate lead at concentration in tissue that exceed those in water. Lead accumulation in marine fish tends to be in bone so that whole fish levels are often higher than those in muscle or viscera (Bodek et al., 1988). Both invertebrate and vertebrate freshwater organisms indicate bioconcentration of lead. In freshwater invertebrates, highest concentrations are in viscera and in freshwater vertebrates highest concentrations are in mucus.

- 1000 reported by Bodek et al. (1988) as a typical concentration ratio in marine invertebrates relative to water concentration.
- 300 reported by Bodek et al. (1988) as a typical concentration ratio in marine fish relative to water concentration.
- 100,000 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater invertebrates relative to water concentration.
- 300 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater fish relative to water concentration.
- 7 to 100,000 based on 0.00003 mg/L as a geosphere average of ocean-water lead concentration and 0.001 to 15 mg/kg (dry mass) as an average of marine-fish lead concentration reported by Bowen (1979) and our assumed fish dry mass fraction in the range 0.2.

Recommended BCF value, based on the geometric mean and geometric standard deviation reflecting the range of BCF values described above:

$$\log \text{BCF}(\text{fish}) = 2.7 \pm 1.7$$

$$\text{BCF}(\text{fish}) = 500 \times \text{or} \div 50$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle, B_k

Ng (1982) and Stevens (1991) have evaluated several studies investigating the concentration of soluble forms of lead (Pb) in milk relative to the Pb intake in feed.

2.1×10^{-5} to 6.5×10^{-5} d/L is the range of values Ng (1982) reported in studies for uptake to milk from feed based on radioisotope studies.

1.4×10^{-4} to 4.5×10^{-4} d/L is the range of values Ng (1982) reported in studies for uptake to milk from feed based on the naturally occurring stable isotopes of lead.

1.2×10^{-5} to 1.4×10^{-3} d/L is the range of values Stevens (1991) identified in studies investigating the concentration of soluble forms of lead (Pb) in milk, relative to the Pb intake in feed.

4.9×10^{-5} d/L was derived from a study by Vreman et al. (1986) by Stevens (1991) who considered this to be the most reliable estimate of this biotransfer factor.

Recommended biotransfer factor, B_k , for milk based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_k = -4.0 \pm 0.73$$

$$B_k = 0.0001 \times \text{or} \div 5.4$$

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

Ng (1982) and Stevens (1992) have evaluated several studies investigating the concentration of soluble forms of lead (Pb) in meat from cattle, relative to the Pb intake in feed by these cattle.

2×10^{-4} to 2×10^{-3} d/kg is the range of values Ng (1982) reported in studies for uptake to beef from feed.

6×10^{-5} to 1.2×10^{-3} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of lead (Pb) in bovine muscle relative to the Pb intake in feed.

2.4×10^{-3} to 7.3×10^{-1} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of lead (Pb) in bovine kidney relative to the Pb intake in feed.

4.1×10^{-3} to 4.9×10^{-1} d/kg is the range of values Stevens (1992) identified in studies investigating the concentration of lead (Pb) in bovine liver relative to the Pb intake in feed.

1.25×10^{-2} d/kg is the value considered by Stevens (1992) to be the most reasonable estimate of a steady-state biotransfer factor for lead to beef.

Recommended biotransfer factor, B_t , for meat based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_t = -2.3 \pm 1.4$$

$$B_t = 0.0048 \times \text{or} \div 24$$

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for lead are available in the current literature.

Ng (1982) has shown that for the seven elements strontium, rubidium, iodine, cesium, cerium, plutonium, and americium, the 68% confidence interval range of the ratio of egg contents biotransfer to beef biotransfer is $60 \times \text{or} \div 13$. Based this observation, the meat biotransfer above can be used to make an estimate of egg contents biotransfer of $0.3 \times \text{or} \div 13$.

Recommended biotransfer factor, B_e , for eggs:

$$\log B_e = -0.52 \pm 1.1$$

$$B_e = 0.3 \times \text{or} \div 13$$

Contaminant biodegradation factors in soil

Although laboratory experiments have demonstrated lead methylation in lake sediments, there is no evidence of biodegradation of inorganic lead in soils (Bodek et al. 1988). Thus there is no recommended biodegradation factor for inorganic lead compounds in soils.

Media-specific half lives for air, soil, and surface water

There is no evidence that lead and its inorganic compounds react in air, soil, or water in such a way as to increase an existing physical removal of lead from these compartments. Thus the half lives of lead species in these compartments will depend entirely upon the removal rate due to natural physical processes such as deposition and erosion.

Recommended half-lives:

<i>Air</i>	deposition half time
<i>Soil</i>	erosion half time
<i>Water</i>	suspended particle half time

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Nickel (Ni)

Nickel is one of many trace elements that are pervasive in the environment as a result of releases from both human and natural sources. Nickel ores occur primarily in the form of the oxides, silicates, and sulfides and are usually associated with other sulfide, silicate, or arsenide minerals (Bodek et al., 1988). Nickel is obtained commercially from pentlandite and pyrrhotite ores. Pentlandite also contains copper and iron. Nickel belongs to the iron-cobalt group of metals and is chiefly valuable for the alloys it forms. It is extensively used for making stainless steel and other corrosion-resistant alloys. It is also used extensively for making coins. Nickel metal, nickel sulfate, nickel chloride, and nickel cyanide are used in electroplating (Bodek et al., 1988). Other uses of nickel are in batteries and catalysts (Weast et al., 1986). Although nickel can have a valance of +1, +2, +3, or +4, the only oxidation state of importance under environmental conditions is the +2 state (Bodek et al., 1988). Nickel forms a number of salts, including nickel carbonate (NiCO_3), nickel chloride (NiCl_2), nickel hydroxide [$\text{Ni}(\text{OH})_2$], nickel sulfate (NiSO_4), and nickel sulfide (NiS). The environmentally important nickel compounds are the sulfide, hydroxide, and carbonate compounds.

Molecular and atomic weights

- 58.69 g/mol, atomic weight of elemental Ni (Weast et al., 1986).
- 58.71 g/mol, atomic weight of Ni (Bowen, 1979).
- 118.70 g/mol, molecular weight of nickel carbonate, NiCO_3 (Weast et al., 1986).
- 129.60 g/mol, molecular weight of nickel chloride, NiCl_2 (Weast et al., 1986).
- 92.70 g/mol, molecular weight of nickel hydroxide, $\text{Ni}(\text{OH})_2$ (Weast et al., 1986).
- 154.75 g/mol, molecular weight of nickel sulfate, NiSO_4 (Weast et al., 1986).
- 90.75 g/mol, molecular weight of nickel sulfide, NiS (Weast et al., 1986).

Melting points

- 1452 °C for nickel metal, Ni (Stull, 1947).
- 1455 °C for nickel metal, Ni (Weast et al., 1986).
nickel carbonate, NiCO_3 , decomposes before melting, (Weast et al., 1986)
- 1001 °C for nickel chloride, NiCl_2 (Stull, 1947).

848 °C nickel sulfate, NiSO_4 , decomposes before melting (Weast et al., 1986).

797 °C for nickel sulfide, NiS (Weast et al., 1986).

Vapor pressures

2732 °C is the boiling point of nickel metal, Ni (Stull, 1947).

nickel chloride, NiCl_4 , sublimates at 973 °C (Weast et al., 1986).

Stull (1947) reports the following vapor pressures for nickel metal (Ni).

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
1810	1	0.133
1979	5	0.667
2087	10	1.33
2143	20	2.67
2234	40	5.33
2289	60	8.00
2364	100	13.3
2473	200	26.7
2603	400	53.3
2732	760	101

Recommended value:

No recommended vapor pressure for inorganic Nickel, because of the extremely low vapor pressures of Ni and its compounds, a VP of 0 is appropriate.

Solubility in water

The nickel compounds that are environmentally important are the relatively insoluble sulfide, hydroxide, and carbonate compound (Bodek et al., 1988). The only oxidation state of importance for nickel under environmental conditions is +2. Because nickel tends to form complexes with both organic and inorganic ligands in aquatic systems, its apparent solubility in surface water systems and in soil solutions can increase significantly over the values reported below for

solubility in pure water. In an organic-free aquatic system, the predominant Ni species over the pH range 2 to 9 are Ni^{+2} and NiSO_4 .

metal nickel, Ni, is insoluble in water (Weast et al., 1986).

93 mg/L (0.78 mol/m^3) of nickel carbonate (NiCO_3), at 25°C (Weast et al., 1986).

130 mg/L (1.4 mol/m^3) of nickel hydroxide ($\text{Ni}[\text{OH}]_2$), at 20°C (Weast et al., 1986).

293,000 mg/L (1890 mol/m^3) of nickel sulfate (NiSO_4), at 20°C (Weast et al., 1986).

873,000 g/L (5640 mol/m^3) of nickel sulfate (NiSO_4), at 100°C (Weast et al., 1986).

3.6 mg/L (0.039 mol/m^3) of nickel sulfide (NiS), at 18°C (Weast et al., 1986).

Recommended values:

$\text{WS}(\text{Ni metal}) = \sim 0$

$\text{WS}(\text{Ni}^{+2}) = 0.039 \text{ to } 5640 \text{ mol/m}^3$ depending on the presence of inorganic species in the water system.

Henry's law constant

Because of their almost complete speciation in water and extremely low vapor pressures, most nickel compounds do not have measurable or predicted Henry's law constants. However, at low concentrations, the ratio of air to water concentration in air and water environments that are in contact can be estimated as

$$C_w/C_a = A \times v_d / (V_w \times R_w)$$

where C_w is the nickel concentration in a given water body, mol/m^3 ; C_a is the nickel concentration in air above the water body, mol/m^3 ; v_d is the deposition velocity that represents the rate of nickel transfer from air to water, m/d ; A is the contact area between the air and water, m^2 ; V_w is the volume of the water body, m^3 ; and R_w is the first-order rate constant that accounts for all nickel removals from water (i.e. precipitation and deposition), day^{-1} .

Partition coefficients in soils and sediments

200 L/kg reported by Bodek et al. (1988) as a K_d value observed for Ni in clay soils.

Bodek et al. (1988) list ranges of Freundlich isotherm parameters for modeling sorption of nickel in six different soil types, silt loam, sandy loam, loamy sand, sand, clay, and clay loam. The following Freundlich-isotherm derived distribution coefficients, K_d , bracket the range of isotherms developed by Bodek et al. (1988),

$$K_d = S/C = 5.0 C^{0.81}/C \text{ [L/kg]} \quad \text{for loamy-sand soil}$$

$$K_d = S/C = 10 C^{0.99}/C \text{ [L/kg]}$$

$$K_d = S/C = 57 C^{0.57}/C \text{ [L/kg]} \quad \text{for silt-loam soil}$$

$$K_d = S/C = 444 C^{0.96}/C \text{ [L/kg]}$$

$$K_d = S/C = 600 C^{0.95}/C \text{ [L/kg]} \quad \text{for clay soil}$$

$$K_d = S/C = 730 C^{1.03}/C \text{ [L/kg]}$$

where S is the sorbed nickel concentration, mg/kg, and C is nickel concentration in water, mg/L. The figure below illustrate the dependence of the distribution coefficient for nickel on nickel concentration in the water phase based on these Freundlich isotherms.

Recommended value of K_d for nickel in soils and in sediments based on the geometric mean and geometric standard deviation of values considered above:

$$5 \leq K_d \leq 1500 \text{ in soils and sediments}$$

$$\log K_d = 1.9 \pm 0.715 \text{ in soils}$$

$$K_d = 80 \times \text{ or } + 5.2 \text{ in soils}$$

Diffusion coefficient in water

In dilute solutions of ionized species, such as nickel compounds, in which there are no rapid chemical reactions and the solution is isothermal, Bodek et al. (1988) have shown that diffusion coefficients for the anions and cations in solution do not vary greatly and are on the order of $1.5 \times 10^{-9} \text{ m}^2/\text{s}$. The diffusion coefficients of many simple salts generally do not vary by more than a factor of 2 over a range of concentrations and temperatures even though the conductivities can vary greatly (Bodek et al., 1988).

Recommended value:

$$D_{\text{water}} = 1.3 \times 10^{-4} \text{ m}^2/\text{d} \text{ or } 1.5 \times 10^{-9} \text{ m}^2/\text{s} \times \text{or} + 2 \text{ for } 0^\circ\text{C} \leq T \leq 40^\circ\text{C}$$

Diffusion coefficient in air

Because of the extremely low vapor pressure of nickel and inorganic nickel compounds, these chemical species are not likely to be found in the gas phase of the environment. There is no need for a diffusion coefficient in air and, thus no value is recommended.

Bioconcentration factors for plant tissue relative to soil concentration $\text{kg}(\text{soil})/\text{kg}(\text{plant fresh mass})$, K_{ps}

Nickel is an essential trace element for plants and animals (Mertz, 1981). Root uptake of nickel as Ni^{+2} occurs through water uptake by roots (Bodek et al. (1988).

0.019 based on a vegetation-fresh-mass-to-soil coefficient described by Ng (1982).

0.006 to 0.018 based on a soil-to-plant-dry-mass coefficient of 0.06 used by Baes et al. (1984) for the vegetative and non-vegetative portions of food crops and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

0.0017 to 0.0051 based on a soil-to-plant-dry-mass coefficient of 0.017 used by Bennett (1982) for land plants and foods and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

0.002 to 0.03 based on 50 mg/kg as the geosphere average of soil nickel concentration and 1 to 5 mg/kg (dry mass) as a geosphere average of land-plant nickel concentration reported by Bowen (1979) and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

0.00004 to 0.024 based on 50 mg/kg as the geosphere average of soil nickel concentration and 0.02 to 4 mg/kg (dry mass) as a geosphere average of edible-plant nickel concentration reported by Bowen (1979) and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

$0.0008 \times \text{or} + 29$ based on 5 to 5000 mg/kg as the range of background soil nickel levels and 0.1 to 5 mg/kg (dry mass) as the range of background plant levels reported by Bodek et al. (1988) and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

$0.0008 \times \text{or} + 20$ based on a 4 to 230 mg/kg as the range of background soil nickel levels and 0.01 to 3 mg/kg (dry mass) as the range of plant levels reported by Bennett (1982) and our assumed plant dry-mass fraction in the range 0.1 to 0.3.

$0.0034 \times \text{or} + 2.2$ is the partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} (Dreicer et al. 1984).

Recommended value of K_{ps} based on the log mean of the ranges of values considered above,

$$\log K_{ps} = -2.6 \pm 1.1$$

$$K_{ps} = 0.0024 (\times \text{or} + 12) \text{ kg}(\text{soil})/\text{kg}(\text{plant fresh mass})$$

Steady-state bioconcentration factors for plant leaf relative to air concentration

According to Bodek et al. (1988), airborne deposition is believed to contribute to concentrations of nickel found in plant leaves. At low concentrations, the ratio of plant leaf concentration to air concentration when air and plant environments are in contact, can be estimated as

$$C_p/C_a = A \times v_d / (V_p \times R_p)$$

where C_p is nickel concentration in the plants in contact with contaminated air, mol/m³; C_a is the nickel concentration in air above the plants, mol/m³; v_d is the deposition velocity that represents the rate of nickel transfer from air to plant surfaces, m/d; A is the contact area between the air and plants, m²; V_p is the volume of the plants compartment, m³; and R_p is the first-order rate constant that accounts for all nickel removals from plants (i.e. wash-off, biodegradation, etc.), day⁻¹.

Bioconcentration factors for fish relative to water/or sediment concentrations

- 250 reported by Bodek et al. (1988) as a typical concentration ratio in marine invertebrates relative to water concentration.
- 100 reported by Bodek et al. (1988) as a typical concentration ratio in marine fish relative to water concentration.
- 100 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater invertebrates relative to water concentration.
- 100 reported by Bodek et al. (1988) as a typical concentration ratio in freshwater fish relative to water concentration.
- 34 to 1400 based on 0.00058 mg/L as a geosphere average of ocean-water nickel concentration and 0.1 to 4 mg/kg (dry mass) as an average of marine-fish nickel concentration reported by Bowen (1979) and our assumed fish dry-mass fraction of 0.2.

Recommended BCF value, based on the geometric mean and geometric standard deviation reflecting the range of BCF values described above:

$$\log \text{BCF}(\text{fish}) = 2.2 \pm 0.55$$

$$\text{BCF}(\text{fish}) = 160 \times \text{or} + 3.5$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle, B_k

0.001 to 0.0067 d/L is the range of values of uptake to milk from feed based on radioisotope studies reported by Ng (1982).

Stevens (1991) evaluated several studies investigating the concentration of soluble forms of Ni in milk relative to the Ni intake in feed and found insufficient information available to calculate an accurate biotransfer factor for nickel.

Recommended biotransfer factor, B_k , for milk based on the geometric mean and geometric standard deviation reflecting the value range above:

$$\log B_k = -2.6 \pm 0.24$$

$$B_k = 0.0025 (\times \text{ or } \div 1.7) \text{ d/L}$$

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

0.002 ($\times$ or $\div 1.7$) d/kg are the geometric mean and geometric standard deviation of the meat-diet biotransfer factor reported by (1982).

0.006 d/kg is the value considered by Stevens (1991) to be the most reasonable estimate of a steady-state biotransfer factor for nickel to bovine muscle.

Recommended biotransfer factor, B_t , for meat based on the geometric mean and geometric standard deviation reflecting the range of values above:

$$\log B_t = -2.6 \pm 0.23$$

$$B_t = 0.003 \times \text{ or } \div 1.7$$

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for nickel are available in the current literature.

Ng (1982) has shown that for the seven elements strontium, rubidium, iodine, cesium, cerium, plutonium, and americium, the ratio of egg contents biotransfer to beef biotransfer is $60 \times$ or $\div 13$. Based this observation, the meat biotransfer above can be used to make an estimate of egg contents biotransfer of $0.18 \times$ or $\div 13$.

Recommended biotransfer factor, B_e , for eggs:

$$\log B_e = -0.74 \pm 1.1$$

$$B_e = 0.18 \times \text{or} \div 13$$

Contaminant biodegradation factors in soil

There is no evidence of biodegradation of inorganic nickel in soils and sediments (Bodek et al. 1988). Thus, there is no recommended biodegradation factor for inorganic nickel compounds in soils.

Media-specific half lives for air, soil, and surface water

There is no evidence that inorganic nickel compounds react in air, soil, or water in such a way as to increase an existing physical removal of nickel from these compartments. Thus the half lives of nickel species in these compartments will depend entirely upon the removal rate due to natural physical processes such as deposition and erosion.

Recommended half-lives:

Air deposition half life

Soil erosion half life

Water suspended particle half life

References for Nickel

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Tetrachloroethylene (PCE)

Other names: Perchloroethylene, ethylene tetrachloride, tetrachloroethene.

CAS Registry Number: 127-18-4

Tetrachloroethylene (PCE) is released to air and water from its uses as a solvent, dry cleaning agent, and degreasing agent. PCE is used as a solvent for fats, greases, waxes, rubber, and decaffeinating coffee. It is used to remove soot from industrial boilers. PCE is used as a heat-transfer medium and also used in the manufacture of fluorocarbon refrigerants, paint removers, and printing inks. Additionally, in manufacturing, PCE is a primary source for the preparation of trichloroacetic acid. PCE typically enters the atmosphere as a fugitive emission from these industrial uses.

Formula: C_2Cl_4

Molecular weight

165.82 (Howard et al., 1990)

165.83 (Verschueren, 1983; Weast et al., 1986; Weast and Grasselli, 1989)

165.85 (Windholz et al., 1983)

Melting Point

-19 °C (Howard et al., 1990; Weast and Grasselli, 1989)

-22.7 °C (Verschueren, 1983)

-22 °C (Windholz et al., 1983)

Octanol-water partition coefficient (K_{ow})

339 based on a log K_{ow} of 2.53 reported by Hansch and Leo (1987) from a value measured by and reported in Chiou et. al. (1977)

398 based on a log K_{ow} of 2.60 reported by Hansch and Leo (1987) from an unpublished value measured by G. Gould and C. Hansch. This value is also cited by Verschueren (1983).

- 759 based on a log K_{ow} of 2.88 reported by Hansch and Leo (1987) based on a value measured by and reported in Banerjee et. al. (1980)
- 759 based on a log K_{ow} of 2.88 reported by Hansch and Leo (1987) based on a value measured by and reported in Banerjee et. al. (1980)
- 2510 based on a log K_{ow} of 3.40 reported by Hansch and Leo (1987) from an unpublished value measured by G. Gould and C. Hansch. This value is also cited by Howard et al. (1990), who attribute the value to Hansch and Leo (1985).
- 6030 based on a log K_{ow} of 3.78 reported by Hansch and Leo (1987) based on a value measured by and reported in Kenaga and Goring (1980).

Recommended value, based on the log-mean value of the 6 measured values reported above:

$$\log K_{ow} = 3.0 \pm 0.5$$

$$K_{ow} = 1000 \times \text{or} \div 3$$

Vapor pressure at standard temperatures

2.47 kPa at 25 °C reported by Howard et al. (1990), who attribute this value to Daubert and Danner (1985).

The Merck Index (Windholz et al., 1983) reports the boiling point of PCE as 121 °C

Stull (1947) reports the following vapor pressures (VPs) for PCE.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
2.4	5	0.667
13.8	10	1.33
26.3	20	2.67
40.1	40	5.33
49.2	60	8.00
61.3	100	13.3
79.8	200	26.7
100	400	53.3
121	760	101

Interpolating from this data gives VP at 25 °C = 2.46 kPa

Verschueren (1983) reports the following vapor pressures for PCE.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
20	14	1.87
30	24	3.20
40	45	6.00
121.4	760	101

Interpolating from this data give VP at 25 °C = 2.57 kPa

The following Antoine equations have been published for estimating the vapor pressure of PCE in kPa

$$\log_{10}(\text{VP}) = 6.195 - \frac{1446}{224.1 + T} \quad \text{for } 28^\circ\text{C} < T < 108^\circ\text{C} \text{ from Boublik et al (1984),}$$

which gives VP = 2.45 kPa at 25° C;

$$\log_{10}(\text{VP}) = 6.103 - \frac{1388}{217.6 + T} \quad \text{for } 37^\circ\text{C} < T < 120^\circ\text{C} \text{ from Boublik et al (1984),}$$

which gives VP = 2.41 kPa at 25° C; and

$$\log_{10}(\text{VP}) = 6.102 - \frac{1387}{217.5 + T} \quad \text{for } 37^\circ\text{C} < T < 120^\circ\text{C} \text{ from Dean (1985),}$$

which also gives VP = 2.41 kPa at 25° C.

The Antoine equation above in the temperature range 28 °C < T < 108°C proposed by Boublik et al. (1984) for VP versus temperature is plotted below.

Recommended value for the temperature range -10 to 40 °C, based on the Antoine equation of Boublik et al. (1984) above:

$$\text{VP(kPa)} = 10^{[6.195 - 1446/(224.1 + T)]} \pm 0.07 \text{ for } -10^\circ\text{C} < T < 40^\circ\text{C}$$

$$\text{VP(kPa)} = 2.45 \pm 0.07 @ 25^\circ\text{C}$$

Solubility in water

150 mg/L at 25 °C reported by Verschueren (1983).

162 mg/L approximate solubility reported by *The Merck Index* (Windholz et al., 1983).

150.3 mg/L at 25 °C reported by Howard et al. (1990), who attribute this value to Horvath (1982).

130 mg/L at 1.5 °C reported as ppm by wt by Dilling (1977). [As cited in Horvath (1982)].

75 mg/L at 15 °C reported as wt % by Antropov et al. (1972). [As cited in Horvath (1982)].

87 mg/L at 20 °C reported as wt % by Antropov et al. (1972). [As cited in Horvath (1982)].

120 mg/L at 20 °C reported as ppm by wt by Dilling (1977). [As cited in Horvath (1982)].

200 mg/L at 20 °C reported as wt % by du Pont (1966). [As cited in Horvath (1982)].

- 200 mg/L at 20 °C reported as wt % by Marsden (1963). [As cited in Horvath (1982)].
- 210 mg/L at 20 °C reported by Moiseeva et al. (1977). [As cited in Horvath (1982)].
- 150 mg/L at 20 °C reported as ppm by wt by Pearson and McConnell (1975). [As cited in Horvath (1982)].
- 150 mg/L at 20 °C reported as ppm by wt by Selenka and Bauer (1978). [As cited in Horvath (1982)].
- 100 mg/L at 25 °C reported as g/g-water by Valluad et al. (1957). [As cited in Horvath (1982)].
- 140 mg/L at 25 °C reported as ppm by wt by Dilling (1977). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by Archer and Stevens (1977). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as wt % by Gladis (1960). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by Hancock (1973). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by Hooker Chemical Corp. (1966). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported by Imperial Chemical Industries (1972). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported by as wt % by Interdyne, Inc. (1976). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by Kirk-Othmer (1964). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by McGovern (1943). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as wt % by Miller (1969). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as wt % by Mitchell and Smith (1977). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as wt % by Nathan (1978). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by O'Connel (1963). [As cited in Horvath (1982)].

- 150 mg/L at 25 °C reported as g/g-water by Pittsburgh Plate Glase Ind. (1971). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as wt % by Riddick and Bunger (1970). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported by Schwarzenbach et al. (1979). [As cited in Horvath (1982)].
- 150 mg/L at 25 °C reported as g/g-water by Sconce (1962). [As cited in Horvath (1982)].
- 189 mg/L at 25 °C reported by Wright and Schaffer (1932). [As cited in Horvath (1982)].
- 200 mg/L at 25 °C reported as wt % by Coca and Diaz (1980). [As cited in Horvath (1982)].
- 200 mg/L at 25 °C reported as wt % by Gunther et al. (1968). [As cited in Horvath (1982)].
- 400 mg/L at 25 °C reported as ppm by wt by Chiou et al. (1977). [As cited in Horvath (1982)].
- 400 mg/L at 25 °C reported as wt % by Matthews (1975, 1979). [As cited in Horvath (1982)].
- 480 mg/L at 25 °C reported as mol/L-solution by Banerjee et al. (1980). [As cited in Horvath (1982)].
- 1000 mg/L at 25 °C reported as wt % by Ethyl Corp. (1958). [As cited in Horvath (1982)].
- 151 mg/L at 26 °C reported as wt % by Antropov et al. (1972). [As cited in Horvath (1982)].
- 166 mg/L at 40 °C reported as wt % by Simonov et al. (1974). [As cited in Horvath (1982)].

From the information above, Horvath (1982) has constructed the following polynomial fit for the dependence of PCE solubility (in wt %) on temperature (T) in °C in the range 0 to 80 °C

$$WS(\text{wt } \%) = 1.497 \times 10^{-2} - 7.801 \times 10^{-6} T - 5.1403 \times 10^{-7} T^2 + 3.694 \times 10^{-8} T^3 \\ \pm 0.001 \text{ (standard error of the estimate)}$$

which gives

$$WS = 0.015 \pm 0.0076 \text{ (wt } \%) \text{ at } 25 \text{ } ^\circ\text{C} \\ = 150 \pm 76 \text{ mg/L at } 25 \text{ } ^\circ\text{C} \\ = 0.91 \pm 0.46 \text{ mol/m}^3 \text{ at } 25 \text{ } ^\circ\text{C}$$

The dependence of PCE solubility in water on temperature as given by this formula is plotted below.

The standard deviation in the water solubility at 25 °C is based on the coefficient of variation in the average solubility of PCE at 25 °C as derived from the values listed above instead of the standard error of the estimate as reported by Horvath (1982) in the correlation of water solubility above. (The standard error of the estimate is based on the estimation of the average solubility as a function of temperature and does not reflect the variation of solubility with temperature at any given temperature value. As reflected by the range of measured solubilities listed above, the coefficient of variation of solubility for PCE is 0.508 at 25 °C and 0.3 at 20 °C.

Recommended values of solubility versus temperature, T in °C, based on Horvath's (1982) analysis:

$$\text{WS(mg/L)} = 149.7 - 0.07801 T - 5.1403 \times 10^{-3} T^2 + 3.694 \times 10^{-4} T^3 \\ \pm 10 \text{ mg/L for } 0^\circ\text{C} < T < 60^\circ\text{C}$$

$$\text{WS(mol/m}^3\text{)} = 0.9029 - 4.7051 \times 10^{-4} T - 3.100 \times 10^{-5} T^2 + 2.228 \times 10^{-6} T^3 \\ \pm 0.060 \text{ mol/m}^3 \text{ for } 0^\circ\text{C} < T < 60^\circ\text{C}$$

$$\text{WS(mg/L)} = 150 \pm 76 \text{ mg/L @ } 25^\circ\text{C}$$

$$\text{WS(mol/m}^3\text{)} = 0.91 \pm 0.46 \text{ mol/m}^3 \text{ @ } 25^\circ\text{C}$$

Henry's law constant (dimensionless form, i.e. H/RT)

- 0.48 reported at 20 °C by Lincoff and Gossett (1984) based on batch stripping. [Also cited in Mackay et al. (1993)].
- 0.54 reported at 20 °C by Lincoff and Gossett (1984) based on EPICS. [Also cited in Mackay et al. (1993)].
- 0.54 reported at 20 °C by Yurteri et al. (1987) based on EPICS. [Also cited in Mackay et al. (1993)].
- 0.55 reported at 20 °C by Gossett (1987) based on EPICS. [Also cited in Mackay et al. (1993)].
- 0.59 reported at 20 °C by Munz and Roberts (1987) based on multiple equilibrium. [Also cited in Mackay et al. (1993)].
- 0.63 reported at 20 °C by Munz and Roberts (1982) based on batch stripping. [Also cited in Mackay et al. (1993)].
- 0.67 reported at 20 °C by Mackay et al. (1979) based on batch stripping. [Also cited in Mackay et al. (1993)].
- 0.70 reported at 20 °C by Ashworth et al. (1986) based on EPICS. [Also cited in Mackay et al. (1993)].
- 0.82 reported at 20 °C by McConnell et al. (1975). [Also cited in Mackay et al. (1993)].

0.85 ± 0.43 obtained by taking the ratio of VP/WS divided by RT at 20 °C, where VP and WS are the values recommended above.

0.66 reported at 25 °C by Leighton and Calo (1981) based on concentration-ratio gas chromatography. [Also cited in Mackay et al. (1993)].

1.17 reported at 25 °C by Urano and Murata (1985) based on the adsorption-isotherm method. [Also cited in Mackay et al. (1993)].

0.75 reported at 25 °C by Gossett (1987) based on EPICS. [Also cited in Mackay et al. (1993)].

0.71 reported at 25 °C by Munz and Roberts (1987). [Also cited in Mackay et al. (1993)].

0.55 reported at 25 °C by Tancrede and Yanagisawa (1990) based on purge and trap gas chromatography. [Also cited in Mackay et al. (1993)].

0.90 ± 0.46 obtained by taking the ratio of VP/WS divided by RT at 25 °C, where VP and WS are the values recommended above.

Recommended value at 20 °C based on the arithmetic mean of the nine measured values above:

$$H/RT = 0.61 \pm 0.10 @ 20\text{ °C}$$

Recommended value at 25 °C based on the arithmetic mean of the five measured values above:

$$H/RT = 0.77 \pm 0.24 @ 25\text{ °C}$$

Plotted below is the dimensionless Henry's law constant H/RT versus temperature as derived from the ratio of VP/WS/RT using the temperature-dependent expressions for VP and WS presented above.

Organic-carbon partition coefficient (K_{oc})

- 75 derived from a $\log K_{om}$ of 1.64 for untreated B_t-horizon Marlette soil reported at 25 °C by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1993)].
- 86 derived from a $\log K_{om}$ of 1.70 for untreated A-horizon Marlette soil reported at 25 °C by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1993)].
- 110 (or $\log K_{oc} = 2.04$) reported at 25 °C by Schwarzenbach and Westall (1981). [Also cited in Howard et al. (1990) and in Mackay et al. (1993)].
- 209 (or $\log K_{oc} = 2.32$) reported at 25 °C by Chiou et al. (1979). [Also cited in Mackay et al. (1993)].
- 281 (or $\log K_{oc} = 2.45$) reported at 25 °C for surface soil by Pignatello (1990). [Also cited in Mackay et al. (1993)].
- 344 derived from a $\log K_{om}$ of 2.30 for A-horizon Marlette soil treated with DDTMA reported at 25 °C by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1993)].

- 363 (or $\log K_{oc} = 2.56$) reported at 25 °C for soil by Chiou et al. (1988). [Also cited in Mackay et al. (1993)].
- 437 (or $\log K_{oc} = 2.64$) reported at 20 °C for soil, sand, and loess by Grathwohl (1990). [Also cited in Mackay et al. (1993)].
- 626 derived from a $\log K_{om}$ of 2.56 for A-horizon Marlette soil treated with HDTMA reported at 25 °C by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1993)].
- 750 derived from a $\log K_{om}$ of 2.64 for B_t-horizon Marlette soil treated with DDTMA reported at 25 °C by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1993)].
- 970 derived from a $\log K_{om}$ of 2.75 for B_t-horizon Marlette soil treated with HDTMA reported at 25 °C by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1993)].
- 1950 (or $\log K_{oc} = 3.29$) reported at 20 °C for weathered shale and mudrock by Grathwohl (1990). [Also cited in Mackay et al. (1993)].
- 3980 (or $\log K_{oc} = 3.60$) reported at 25 °C for Borden organic phase with no mineral sorption by Ball and Roberts (1991). [Also cited in Mackay et al. (1993)].
- 10700 (or $\log K_{oc} = 4.03$) reported at 20 °C for unweathered shale and mudrock by Grathwohl (1990). [Also cited in Mackay et al. (1993)].

Recommended value, based on the log-mean value of the 13 measured values reported above; (the high K_{oc} value reported for unweathered shale and mudrock is excluded because it is assumed not be relevant for soils):

$$\log K_{oc} = 2.6 \pm 0.5$$

$$K_{oc} = 400 \times \text{or} + 3.2$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

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$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}} .$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the Le Bas incremental method as described in Lyman et al. (1990). With the molecular volume V_x of PCE equal to 111 cm³/mol, this expression gives

Recommended value:

$$D_{\text{water}} = 3.0 \times 10^{-7} T \text{ m}^2/\text{d} = 8.8 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 1.0 \times 10^{-9} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m²/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of PCE of 111 cm³/mol and a molecular weight of 166 g/mol, the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 3.1 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.66 \text{ m}^2/\text{d} \text{ or } 7.6 \times 10^{-6} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C} .$$

Bioconcentration factors for plant tissue concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for PCE in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} is equal to 0.0034 kg(soil)/kg(plant) with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh-mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, mg/kg[fresh mass], to contaminant concentration in soil solution, mg/L) for PCE as

$$RCF = 0.82 + 0.03 K_{ow}^{0.77} = 3.4 \text{ to } 15$$

When this factor is divided by the sorption coefficient, $K_D = f_{oc} \times K_{oc} = (0.01 \text{ to } 0.02) \times K_{oc}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg(fresh mass) to contaminant concentration in soil solids, mg/kg, which we refer to as $K_{ps}(\text{roots})$ and estimate it as being in the range

$$K_{ps}(\text{roots}) = 0.04 \text{ to } 20$$

Based on the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

(recommended range for root crops)

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 3.8 \text{ to } 38 \text{ (reflecting the range in } K_{oc})$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for the total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 0.14 \times \text{or} \div 5.3 \text{ (recommended value for exposed produce reflecting estimation error)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for PCE in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air partition coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{m^3}{kg} = 0.02 m^3/kg \times \text{or} \pm 2.2$$

(recommended value).

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

- 39 (or log BCF of 1.59) reported for trout muscle by Neely et al. (1974). [Also cited in Mackay (1982), in Howard et al. (1990), and in Mackay et al. (1993)].
- 49 (or log BCF of 1.69) reported for bluegill sunfish by Barrows et al. (1980). [Also cited in Howard et al. (1990) and in Mackay et al. (1993)].
- 49 (or log BCF of 1.69) reported for bluegill sunfish by Veith et al. (1980). [Also in Mackay et al. (1993)].
- 62 (or log BCF of 1.79) reported for rainbow trout by Saito et al. (1992). [Also in Mackay et al. (1993)].
- 115 (or log BCF of 2.06) reported for rainbow trout by Veith and Kosian (1983). [Also in Mackay et al. (1993)].
- 16 to 144 Based the $\pm$ one-standard-deviation range of the K_{ow} values above and the estimation method based on K_{ow} of Mackay (1982).

Recommended BCF value, based on the arithmetic mean values of the five measured values and the predicted range of values for log BCF above:

$$\log BCF(\text{fish}) = 1.74 \pm 0.3$$

$$BCF(\text{fish}) = 55 \times \text{or} \pm 2$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for toluene are available in the current literature for PCE.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for PCE as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 7.9 \times 10^{-6} \times \text{or} + 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for PCE are available in the current literature.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for PCE as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 2.5 \times 10^{-5} \times \text{or} + 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for PCE are available in the current literature.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for PCE as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 7.9 \times 10^{-3} \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Based on the aqueous aerobic biodegradation half life of PCE measured by Mudder (1981) and by Jensen and Rosenberg (1975), Howard et al. (1991) estimate the soil half life due to aerobic degradation to be in the range of 180 to 360 d. [This range is also cited in Mackay et al. (1993)]. This range corresponds to an aerobic biodegradation rate constant in the range 0.00193 to 0.00385 d⁻¹. The anaerobic half life of PCE has been estimated to be in the range 100 to 1640 d by Howard et al. (1991) based on anaerobic screening test data from Bouwer et al. (1981). This range corresponds to an anaerobic biodegradation rate constant in the range 0.000423 to 0.0069 d⁻¹.

Recommended soil biodegradation rate constants, based on the log mean and log range of the soil half life ranges above:

aerobic soil biodegradation rate constant = $0.0027 \text{ d}^{-1} \times \text{or} + 1.2$

anaerobic soil biodegradation rate constant = $0.0017 \text{ d}^{-1} \times \text{or} + 2.2$

Media-specific half lives for air, soil, and surface water

- Air.* Based on measurements by Atkinson (1985) of the vapor-phase reaction of PCE with hydroxyl radicals, Howard et al. (1991) estimate the half life of PCE in lower atmosphere is in the range of 16 to 160 d. [This range is also cited in Mackay et al. (1993).] Based on the rate of disappearance of PCE due to reaction with hydroxyl radicals, Yung et al. (1975) report a half-life of 10 d. [This range is also cited in Mackay et al. (1993)].
- Soil* Based on the aqueous aerobic biodegradation half life of PCE measured by Mudder (1981) and by Jensen and Rosenberg (1975), Howard et al. (1991) estimate the soil half life due to aerobic degradation to be in the range of 180 to 360 d. [This range is also cited in Mackay et al. (1993)]. The anaerobic half life of PCE has been estimated to be in the range 100 to 1640 d by Howard et al. (1991) based on anaerobic screening test data from Bouwer et al. (1981).
- Water* Based on the aqueous aerobic river "die-away" test data measured by Mudder (1981) and on saltwater grab-sample data by Jensen and Rosenberg (1975), Howard et al. (1991) estimate the surface-water half life due to aerobic degradation to be in the range of 180 to 360 d. [This range is also cited in Mackay et al. (1993).] Based on the concentration reduction between sample points on the Rhine River and a lake in the Rhine basin, Zoetemann et al. (1980) estimate respective PCE half lives to be 10 and 32 d. These values are cited in Mackay et al. (1993) and in Howard et al. (1990). These latter rate constants reflect processes other than biodegradation, such as volatilization and deposition.

Recommended half lives (in days), based on the geometric mean of the half-life range and the geometric range of the values, 32 to 360 (the lowest value is excluded because of its likely association with transport processes:

Air 40 d $\times$ or $\div$ 2.2

Soil 404 d $\times$ or $\div$ 2.2

Water 130 d $\times$ or $\div$ 3.5

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Tetrachloroethylene

Toluene

Other names: Methyl benzene, phenylmethane, toluol, methyl benzol., methacide

CAS Registry Number: 108-88-3

Toluene is used in the manufacture of benzene derivatives, saccharin, medicines, dyes, perfumes, detergents and explosives. Also, it is used in solvent recovery plants, as a component of gasoline. Additionally, toluene is a solvent for paints and coatings, for gums, resins, and rubber, and it is used as an adhesive solvent in plastic toys. Toluene is released to the atmosphere principally from the volatilization of petroleum fuels and toluene-based solvents and thinners, and from motor-vehicle exhaust. Toluene is obtained mainly from petroleum refining and coal tar distillation. Natural sources of toluene are coal tar, crude oil, volcanoes and forest fires.

Formula: C₇ H₈

Molecular weight

92.1 °C (Verschueren, 1983)

92.13 °C (Weast et al., 1986; Mackay et al., 1992; Howard et al., 1990; Windholz et al., 1983)

Melting Point

-95 °C (Weast et al., 1986; Mackay et al., 1992; Howard et al., 1990)

Octanol-water partition coefficient (K_{ow})

129 derived from a log K_{ow} of 2.11 reported by Hansch and Leo (1985) based on the value measured by Rogers and Cammarata (1969). [Also cited in Mackay et al. (1992)].

162 derived from a log K_{ow} of 2.21 reported by Hansch and Leo (1985) based on the value measured by Banerjee et al. (1980). [Also cited in Mackay et al. (1992)].

- 389 derived from a log K_{ow} of 2.59 based on the value measured by Hanai et al. (1981). [Also cited in Mackay et al. (1992)].
- 407 derived from a log K_{ow} of 2.61 reported by Hansch and Leo (1985) based on the value measured by Tayar et al. (1984).
- 417 derived from a log K_{ow} of 2.62 based on the value measured by Miyake and Terada (1982). [Also cited in Mackay et al. (1992)].
- 447 derived from a log K_{ow} of 2.65 reported by Hansch and Leo (1985) based on the value measured by Tewari et al. (1982a). [Also cited in Mackay et al. (1992)].
- 447 derived from a log K_{ow} of 2.65 as measured by Wasik et al. (1983). [Also cited in Mackay et al. (1992)].
- 447 derived from a log K_{ow} of 2.65 as measured by Eadsforth and Moser (1983). [Also cited in Mackay et al. (1992)].
- 447 derived from a log K_{ow} of 2.65 as measured by Schantz and Martire (1987). [Also cited in Mackay et al. (1992)].
- 479 derived from a log K_{ow} of 2.68 reported by Hansch and Leo (1985) based on the value measured by Nahum and Horvath (1980). [Also cited in Mackay et al. (1992)].
- 490 derived from a log K_{ow} of 2.69 reported by Hansch and Leo (1985) based on the value measured by Fujita et al. (1964). [Also cited in Verschueren (1983) and in Mackay et al. (1992)].
- 525 derived from a log K_{ow} of 2.72 as measured by Garst and Wilson (1984). [Also cited in Mackay et al. (1992)].
- 537 derived from a log K_{ow} of 2.73 reported by Hansch and Leo (1985) based on the value measured by Church and Hansch at Pomona College in Claremont, CA (unpublished data). [Also cited in Howard et al. (1990)].
- 550 derived from a log K_{ow} of 2.74 as measured by Hafkansch and Tomlinson (1983). [Also cited in Mackay et al. (1992)].
- 602 derived from a log K_{ow} of 2.78 as measured by Hammers et al. (1982). [Also cited in Mackay et al. (1992)].
- 603 derived from a log K_{ow} of 2.59 as measured by Burkhard et al. (1985). [Also cited in Mackay et al. (1992)].
- 611 derived from a log K_{ow} of 2.786 as measured by De Bruijn et al. (1989). [Also cited in Mackay et al. (1992)].
- 631 derived from a log K_{ow} of 2.8 reported by Hansch and Leo (1985) based on a private communication from M. Tichy and K. Bocek.

- 645 derived from a log K_{ow} of 2.81 as measured by Doucette and Andren (1988). [Also cited in Mackay et al. (1992)].
- 759 derived from a log K_{ow} of 2.88 as measured by Eadsforth and Moser (1983). [Also cited in Mackay et al. (1992)].
- 779 derived from a log K_{ow} of 2.89 as measured by Rapaport and Eisenreich (1984). [Also cited in Mackay et al. (1992)].
- 870 derived from a log K_{ow} of 2.94 reported by Hansch and Leo (1985) based on the value measured by Konemann et al. (1979).
- 933 derived from a log K_{ow} of 2.97 as measured by McDuffie (1981). [Also cited in Mackay et al. (1992)].
- 1000 derived from a log K_{ow} of 3.00 as measured by De Kock and Lord (1987). [Also cited in Mackay et al. (1992)].

Recommended value, based on the log-mean value of the 24 measured values reported above:

$$\log K_{ow} = 2.70 \pm 0.20$$

$$K_{ow} = 501 \times \text{or} \div 1.6$$

Vapor pressure at standard temperatures

3.79 kPa at 25 °C reported by Daubert and Danner (1985). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].

The Merck Index (Windholz et al., 1983) reports a boiling point of 110.6 °C

Stull (1947) reports the following vapor pressures for toluene.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
-4.4	5	0.667
6.4	10	1.33
18.4	20	2.67
31.8	40	5.33
40.3	60	8.00
51.9	100	13.3
69.5	200	26.7
89.5	400	53.3
110.6	760	101

Interpolating from the above data gives VP at 25 °C = 3.69 kPa

Verschueren (1983) reports the following vapor pressures for toluene.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
6.4	10	1.33
20	22	2.93
31.8	40	5.33
110.6	760	101

Interpolating from this data give VP at 25 °C = 3.71 kPa

The following Antoine equations have been published for estimating the vapor pressure of toluene in kPa

$$\log_{10}(\text{VP}) = 6.0844 - \frac{1347.6}{219.79 + T} \quad \text{for } 35^\circ\text{C} < T < 110^\circ\text{C} \quad \text{from Boublik et al. (1984),}$$

which gives VP = 3.79 kPa at 25° C and

$$\log_{10}(\text{VP}) = 6.0795 - \frac{1344.8}{219.48 + T} \quad \text{for } 6^\circ\text{C} < T < 137^\circ\text{C} \quad \text{from Wilhoit and Zwolinski (1971) and from Dean (1985),}$$

which also gives VP = 3.79 kPa at 25° C.

The Antoine equation above in the temperature range 6 °C < T < 137°C proposed by Wilhoit and Zwolinski (1971) for VP versus temperature is plotted below.

Recommended value for the temperature range -10 to 40 °C, based on the Antoine equation of Wilhoit and Zwolinski (1971) above:

$$\text{VP(kPa)} = 10^{[6.0795 - 1344.8/(219.48 + T)]} \pm 0.05 \quad \text{for } -10^\circ\text{C} < T < 40^\circ\text{C}$$

Recommended value for the temperature 25 °C, based on the mean of the four values above

$$\text{VP(kPa)} = 3.75 \pm 0.05 @ 25^\circ\text{C}$$

Solubility in water

- 470 mg/L at 16 °C reported by Verschueren (1983).
- 515 mg/L at 20°C reported by Verschueren (1983).
- 479 mg/L at 21 °C measured by Chey and Calder (1972). [Also cited in Mackay et al. (1992)].
- 347 mg/L at 25 °C measured by Booth and Everson (1948). [Also cited in Mackay et al. (1992)].
- 470 mg/L at 25 °C measured by Fühner (1924). [Also cited in Mackay et al. (1992)].
- 488 mg/L at 25 °C measured by Sada et al (1975). [Also cited in Mackay et al. (1992)].
- 500 mg/L at 25 °C measured by Klevens (1950). [Also cited in Mackay et al. (1992)].
- 507 mg/L at 25 °C measured by Rossi and Thomas (1981). [Also cited in Mackay et al. (1992)].
- 515 mg/L at 25 °C measured by McAuliffe (1966). [Also cited in Mackay et al. (1992)].

- 517 mg/L at 25 °C measured by Mackay and Wolkoff (1973) [Also cited in Mackay et al. (1992)].
- 517 mg/L at 25 °C measured by Mackay et al. (1975). [Also cited in Mackay et al. (1992)].
- 520 mg/L at 25 °C measured by Mackay and Shiu (1975). [Also cited in Mackay et al. (1992)].
- 524 mg/L at 25 °C measured by Banerjee (1984). [Also cited in Mackay et al. (1992)].
- 534 mg/L at 25 °C measured by Schwarz (1977). [Also cited in Mackay et al. (1992)].
- 534.8 mg/L at 25 °C measured by Sutton and Calder (1975). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].
- 538 mg/L at 25 °C measured by McAuliffe (1963). [Also cited in Mackay et al. (1992)].
- 538 mg/L at 25 °C measured by Coutant and Keigley (1988). [Also cited in Mackay et al. (1992)].
- 546 mg/L at 25 °C measured by Morrison and Billett (1952). [Also cited in Mackay et al. (1992)].
- 550 mg/L at 25 °C measured by Dreisbach (1955). [Also cited in Mackay et al. (1992)].
- 554 mg/L at 25 °C measured by Price (1976). [Also cited in Mackay et al. (1992)].
- 573 mg/L at 25 °C measured by Polack and Lu (1973). [Also cited in Mackay et al. (1992)].
- 578 mg/L at 25 °C measured by Tewari et al. (1982b). [Also cited in Mackay et al. (1992)].
- 580 mg/L at 25 °C measured by Wasik et al. (1983). [Also cited in Mackay et al. (1992)].
- 580 mg/L at 25 °C measured by Keeley et al. (1988). [Also cited in Mackay et al. (1992)].
- 585 mg/L at 25 °C measured by Tewari et al. (1982c). [Also cited in Mackay et al. (1992)].
- 627 mg/L at 25 °C measured by Bohon and Claussen (1951). [Also cited in Mackay et al. (1992)].
- 627 mg/L at 25 °C measured by Vesala (1974). [Also cited in Mackay et al. (1992)].

570 mg/L at 30 °C measured by Gross and Saylor (1931) [Also cited in Mackay et al. (1992)].

Recommended value based on the arithmetic mean of the measured values above:

$$WS = 535 \pm 55 \text{ mg/L at } 25 \text{ }^{\circ}\text{C}$$

$$5.81 \pm 0.6 \text{ mol/m}^3 \text{ at } 25 \text{ }^{\circ}\text{C}$$

Henry's law constant (dimensionless form, i.e. H/RT)

0.240 reported at 20 °C by Yurteri et al. (1987) based on EPICS. [Also cited in Mackay et al. (1992)].

0.243 reported at 25 °C by Shen (1982). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].

0.244 reported at 25 °C by Keeley et al. (1988) based on concentration ratios. [Also cited in Mackay et al. (1992)].

0.261 reported at 25 °C by Leighton and Calo (1981) based on concentration ratios. [Also cited in Mackay et al. (1992)].

0.261 reported at 25 °C by Garbarini and Lion (1985) based on EPICS. [Also cited in Mackay et al. (1992)].

0.263 reported at 25 °C by Ashworth et al. (1988) based on EPICS. [Also cited in Mackay et al. (1992)].

0.272 reported at 25 °C by Mackay et al. (1979) based on batch stripping. [Also cited in Mackay and Shiu (1981) and Mackay et al. (1992)].

0.274 reported at 25 °C by Suntio et al. (1988) based on batch stripping. [Also cited in Mackay et al. (1992)].

0.275 reported at 25 °C by as an experimental value by Hine and Mookerjee (1975). [Also cited in Mackay et al. (1992)].

0.260 ± 0.03 obtained by taking the ratio of VP/WS divided by RT, where VP and WS are the values recommended above.

Recommended value at 25 °C based on the arithmetic mean of the the values above:

$$H/RT = 0.26 \pm 0.01 @ 25 \text{ }^{\circ}\text{C}$$

The figure below is the plot of the dimensionless Henry's law constant based on the ratio of temperature-dependent vapor pressure to solubility as recommended in sections above.

Organic-carbon partition coefficient (K_{oc})

- 34 derived from a $\log K_{om}$ of 1.29 for untreated soils reported by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1992)].
- 37 based on a K_{om} of 21.7 reported for Wendover silty loam by Nathwani and Phillips (1977) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [Also cited in Howard et al. (1990)].
- 42.3 derived from a $\log K_{om}$ of 1.39 for untreated soils reported by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} value cited in Mackay et al. (1992)].
- 46 based on a K_{om} of 26.9 reported for Vaudreuil sandy loam by Nathwani and Phillips (1977) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [Also cited in Howard et al. (1990)].
- 75 to 131 based on a $\log K_D$ of 0.60 ± 12 measured by Vowles and Mantoura (1987) using HPLC retention factors in soils with 4% organic carbon.

- 77 to 191 reported for soils by Garbarini and Lion (1985). [Also cited in Mackay et al. (1992)].
- 151 measured by Garbarini and Lion (1986) for soil using a headspace technique.
- 160 based on a K_{om} of 93.05 reported for Grimsby silt loam by Nathwani and Phillips (1977) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].
- ~176 based on measurements by Wilson et. al (1981) of retardation velocities in low-organic carbon, sandy soils. [Also cited as 178 in Howard et al. (1990) and in Mackay et al. (1992)].
- 178 derived from a log K_{oc} of 2.25 from reported by Wilson et al. (1981). [Also cited in Mackay et al. (1992)].
- 182 derived from a log K_{oc} of 2.26 reported by Szabo et al. (1990a,b). [Also cited in Mackay et al. (1992)].
- 245 derived from a log K_{oc} of 2.39 reported for soils by Schwarzenbach and Westall (1981). [Also cited in Mackay et al. (1992)].
- 249 to 1340 derived from a log K_{om} of 2.16 to 2.89 for cation-treated soils reported by Lee et al. (1989) and the assumption that $K_{oc} = K_{om} \times 1.724$ (Lyman et al., 1990). [K_{om} values cited in Mackay et al. (1992)].

Recommended value, based on the log-mean value of the 16 measured values reported above:

$$\log K_{oc} = 2.1 \pm 0.41$$

$$K_{oc} = 130 \times \text{or} \div 2.6$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}}$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The

viscosity of water, η_w , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). With the molecular volume V_x of toluene equal to 103 cm³/mol, this expression gives

Recommended value:

$$D_{\text{water}} = 3.1 \times 10^{-7} T \text{ m}^2/\text{d} = 9.2 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 1.1 \times 10^{-9} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m²/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of toluene of 103 cm³/mol and a molecular weight of 92.1 g/mol, the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 3.4 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.72 \text{ m}^2/\text{d} \text{ or } 8.3 \times 10^{-6} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C} .$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for toluene in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, $K_{\text{ps}}^{\text{rain}}$ is equal to 0.0034 kg(soil)/kg(plant) with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, mg/kg[fresh mass], to contaminant concentration in soil solution, mg/L) for toluene as

$$RCF = 0.82 + 0.03 K_{ow}^{0.77} = 3.3 \text{ to } 6$$

When this factor is divided by the sorption coefficient, $K_D = f_{oc} \times K_{oc} = (0.01 \text{ to } 0.02) \times K_{oc}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg(fresh mass) to contaminant concentration in soil solids, mg/kg, which we refer to as $K_{ps}(\text{roots})$ and estimate it as being in the range

$$K_{ps}(\text{roots}) = 0.5 \text{ to } 12$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 7.5 \text{ to } 74 \text{ (recommended range for root crops)}$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 0.21 \times \text{or} + 5.3 \text{ (recommended value for exposed produce)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for toluene in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air partition coefficient of

$$\text{Recommended value, } K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 0.02 \text{ m}^3/\text{kg} \times \text{or} + 2.2$$

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

- 13.2 (or log BCF of 1.12) reported for eels by Ogata and Miyake (1978). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].
- 1.7 (or log BCF of 0.22) reported for Manila clam by Nunes and Benville (1979). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].
- 4.2 (or log BCF of 0.62) reported for mussels by Geyer et al. (1982). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].
- 8.3 (or log BCF of 0.92) reported for goldfish by Ogata et al. (1984). [Also cited in Mackay et al. (1992)].
- 90 (or log BCF of 1.95) reported for golden ide fish by Freitag et al. (1985). [Also cited in Howard et al. (1990) and in Mackay et al. (1992)].
- 98 (or log BCF of 1.99) reported for s. capricornutum by Herman et al. (1991). [Also cited in Mackay et al. (1992)].
- 15 to 39 Based the two-standard-deviation range of the K_{ow} values above and the estimation method based on K_{ow} of Mackay (1982).

Recommended value, based on the log-mean value of the three measured values and one predicted value reported above:

$$\log \text{BCF}(\text{fish}) = 1.14 \pm 0.7$$

$$\text{BCF}(\text{fish}) = 14 \times \text{or} \div 5$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for toluene are available in the current literature.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for toluene as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 4.0 \times 10^{-6} \times \text{or} \div 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for toluene are available in the current literature.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for toluene as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 1.3 \times 10^{-5} \times \text{or} + 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for toluene are available in the current literature.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for toluene as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 4.0 \times 10^{-3} \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Based on the aqueous aerobic biodegradation half life of toluene measured by Wakeham et al. (1983), Howard et al. (1991) estimate the soil half life due to aerobic degradation to be in the range of 4 to 22 d. This range is also cited in Mackay et al. (1992). This range corresponds to an aerobic biodegradation rate constant in the range 0.032 to 0.17 d⁻¹. The anaerobic half life of toluene has been estimated to be in the range 56 to 210 d by Howard et al. (1991) based on anaerobic sediment grab-sample data from Horowitz et al. (1982). This range corresponds to an anaerobic biodegradation rate constant in the range 0.0033 to 0.012 d⁻¹.

Recommended soil biodegradation rate constants, based on the log mean and log range of the soil half life ranges above:

$$\text{aerobic soil biodegradation rate constant} = 0.074 \text{ d}^{-1} \times \text{or} + 1.6$$

$$\text{anerobic soil biodegradation rate constant} = 0.0063 \text{ d}^{-1} \times \text{or} + 1.5$$

Media-specific half lives for air, soil, and surface water

- Air.** Based on measurements of Atkinson (1985), Howard et al. (1991) estimate the half life of toluene in lower atmosphere is in the range of 0.42 to 4.3 d based on photo-oxidation as a removal process. [This range is also cited in Mackay et al. (1992).] Based on the rate of disappearance of toluene due to reaction with hydroxyl radicals, Doyle et al. (1975) report a half life of 0.2 d and Darnall et al. report a half life in the range 0.1 to 1 d.
- Soil** Based on the aqueous aerobic biodegradation half life of toluene measured by Wakeham et al. (1983), Howard et al. (1991) estimate the soil half life due to aerobic degradation to be in the range of 4 to 22 d. This range is also cited in Mackay et al. (1992). The anaerobic half-life of toluene has been estimated to be in the range 56 to 210 d by Howard et al. (1991) based on anaerobic sediment grab-sample data from Horowitz et al. (1982). Anderson et al. (1991) report a disappearance half life of toluene from test soils of less than 2 d. This value is also cited in Mackay et al. (1992).
- Water** Based on the aqueous aerobic biodegradation half life of toluene measured by Wakeham et al. (1983), Howard et al. (1991) estimate the surface-water half life due to aerobic degradation to be in the range of 4 to 22 d. This range is also cited in Mackay et al. (1992).

Recommended half lives (in days), based on the geometric mean of the half lives and the geometric range of the values:

<i>Air</i>	2.1 × or + 3.0 d
<i>Soil</i>	20 × or + 3.8 d
<i>Water</i>	9.4 × or + 1.6 d

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Toluene-2,4-Diisocyanate

Other names: 2,4-diisocyanato-1-methylbenzene; 2,4-diisocyanatoluene; 2,4-TDI; tolyene-2-4-diisocyanate; naconate 100

CAS Registry Number: 584-84-9

Toluene-2,4-diisocyanate (2,4-TDI) is a white liquid used in the manufacture of polyurethane foams and other elastomers. 2,4-TDI constitutes roughly 80% of the commercial toluene diisocyanate (TDI) used in the U.S., the other 20% being the isomer, 2,6-TDI (Howard, 1989). TDI is released to the environment as a fugitive emission from stack exhaust during the production, transport, and use of TDI in the manufacture of polyurethane-foam products. Both 2,4- and 2,6-TDI are reactive with any compound having active hydrogens, i.e. water, acids, alcohols. According to Roegler (1985), the 2,4-isomer is about 1.4 times as reactive with water as the 2,6-isomer. The reactivity of the TDI isomers makes it impossible to define solubilities for these compounds in either water or octanol or in any compound or environmental medium containing water or hydrogen-donor compounds. Because of their high reactivity, TDI isomers are not found in nature. TDI isomers are fully miscible (i.e., infinitely soluble) in alcohol (with decomposition), ether, acetone, carbon tetrachloride, benzene, chlorobenzene, kerosene, and olive oil.

Formula: $C_9H_6N_2O_2$

Molecular weight

174.15 (Windholz et al., 1983)

174.16 (Verschueren, 1983)

174.17 (Howard, 1989)

174.2 (Roegler, 1985)

Melting Point

19.5 to 21.5 °C (Howard, 1989)

Octanol-water partition coefficient (K_{ow})

Because of its reactivity with water, 2,4-TDI cannot be characterized as having an octanol-water partition coefficient. However, because it is fully miscible in olive oil, it is expected to be fully miscible in octanol. If it is fully miscible in octanol, then it has no solubility limit, and it makes little sense to propose an octanol-water partition coefficient. If at low concentrations, TDI behaves as miscible with water before it reacts, then its K_{ow} is essentially unity; otherwise, it is infinite. Based on the QSAR method of fragment contribution as proposed by Leo et al. (1971), one can estimate the K_{ow} for 2,4-TDI, but the miscibility of TDI in organic solvents and its reactivity in water makes such estimates suspect. Nonetheless, such fragment estimating methods indicate that the log K_{ow} of 2,4-TDI is less than zero, indicating a high relative solubility in water.

No recommended K_{ow} . Bioconcentration for TDI cannot be estimated using K_{ow} .

Vapor pressure at standard temperatures

1.33 Pa at 20 °C reported by IARC (1979). [Also cited in Howard (1989).]

The Merck Index (Windholz et al., 1983) and Howard (1989) report a boiling point of 251 °C

Verschuieren (1983) reports the following vapor pressures (VPs) for 2,4-TDI.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (Pa)
20	0.01	1.33
80	1	133
251	760	101,300

Interpolating from this data give VP at 25 °C = 2.3 Pa

The following Antoine equation has been published for estimating the vapor pressure of 2,4-TDI in kPa

$$\log_{10}(\text{VP}) = 6.63416 - \frac{2097.536}{201.33 + T} \pm 0.006 \quad \text{for } 20^\circ\text{C} < T < 170^\circ\text{C} \quad \text{from Boublik et al. (1984),}$$

which gives VP = 2.3 Pa at 25° C.

The relationship between VP and temperature is plotted below, using the Antoine equation shown above.

Recommended values:

$$\text{VP(Pa)} = 10^{[6.63416 - 2097.536/(201.33 + T)] \times \text{or} + 1.014} \quad \text{for } 20^\circ\text{C} < T < 170^\circ\text{C}$$

Recommended value @ 25 °C:

$$\text{VP(Pa)} = 2.3 \pm 0.03 @ 25^\circ\text{C}$$

Solubility in water

No measurements of TDI solubility in water are available in the current literature. Because of its reactivity in water, it is not possible for TDI to estimate water solubility for TDI. As noted above, TDI isomers are fully miscible (i.e.,

infinitely soluble) in alcohol (with decomposition), ether, acetone, carbon tetrachloride, benzene, chlorobenzene, kerosene, and olive oil.

As discussed by Howard (1989), Brochhagen and Grieveson (1984) added 0.5 L of TDI to 20 L of stagnant water and observed the formation of a hard compact crust at the water/TDI interface, as well as the subsequent disappearance of TDI due to hydrolysis.

No recommended solubility. Inter-phase partitioning for TDI cannot be estimated using water solubility.

Henry's law constant

No measurements of Henry's law constants are available for TDI in the current literature. Because of its reactivity in water, it is not possible to estimate Henry's law partitioning for TDI. However, at low concentrations, the ratio of air to water concentration in air and water environments that are in contact can be estimated as

$$C_w/C_a = A \times v_d / (V_w \times R_w)$$

where C_w is the TDI concentration in a given water body, mol/m³; C_a is the TDI concentration in air above the water body, mol/m³; v_d is the deposition velocity that represents the rate of TDI transfer from air to water, m/d; A is the contact area between the air and water, m²; V_w is the volume of the water body, m³; and R_w is the first-order rate constant that accounts for all TDI removals from water (i.e. hydrolysis), day⁻¹.

Organic-carbon partition coefficient (K_{oc})

No measurements of TDI K_{oc} values are available in the current literature. Because of its reactivity in water, it is not possible to make an estimate for TDI of soil-water partitioning.

At low concentrations, the ratio of soil to air concentration in air and soil environments that are in contact, can be estimated as

$$C_s/C_a = A \times v_d / (V_s \times R_s)$$

where C_s is TDI concentration in the soil below a contaminated air mass, mol/m³; C_a is the TDI concentration in air above the soil, mol/m³; v_d is the deposition velocity that represents the rate of TDI transfer from air to land, m/d; A is the contact area between the air and land, m²; V_s is the volume of the soil compartment, m³; and R_s is the first-order rate constant that accounts for all TDI removals from soil (i.e. hydrolysis), day⁻¹.

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}} .$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). With the molecular volume V_x of 2,4-TDI equal to 162 cm^3/mol , this expression gives

Recommended value:

$$D_{\text{water}} = 2.4 \times 10^{-7} T \text{ m}^2/\text{d} = 7.0 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 8.1 \times 10^{-10} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2} ,$$

where the molecular volume, V_x , of 2,4-TDI is 162 cm^3/mol ; the molecular weight of TDI is 174 g/mol; and temperature (T) is expressed in kelvins. Then, the above expression yields:

Recommended value:

$$D_{\text{air}} = 2.6 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.55 \text{ m}^2/\text{d} \text{ or } 6.4 \times 10^{-6} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C} .$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for 2,4-TDI in soils are available in the current literature. The reactive nature of the compound suggests that it is not likely to enter plants through the roots in appreciable quantities.

The partition factor from surface soil to edible plant parts due to rainsplash, K_{ps}^{rain} is equal to 0.0034 kg(soil)/kg(plant) with a CV of 1 (Dreicer et al. 1984). This partition factor yields plant fresh-mass concentration relative to soil concentration.

Recommended bioconcentration for TDI for plant roots relative to soil based on rainsplash only is $K_{ps}^{rain} = 0.0034 \text{ kg(soil)/kg(plant)}$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for 2,4-TDI in air are available in the current literature. At low concentrations, the ratio of plant to air concentration of 2,4-TDI in air and plant environments that are in contact, can be estimated as

$$C_p/C_a = A \times v_d / (V_p \times R_p)$$

where C_p is the TDI concentration in the plants in contact with contaminated air, mol/m³; C_a is the TDI concentration in air above the plants, mol/m³; v_d is the deposition velocity that represents the rate of TDI transfer from air to plant surfaces, m/d; A is the contact area between the air and plants, m²; V_p is the volume of the plants compartment, m³; and R_p is the first-order rate constant that accounts for all TDI removals from plants (i.e. hydrolysis, photolysis, biodegradation, etc.), day⁻¹.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

No reported measurements of fish-water bioconcentration for 2,4-TDI in water or sediments are available in the current literature.

No recommended bioconcentration for TDI between fish and water.

Steady-state biotransfer factors for milk, dairy products, meat and egg concentrations relative to contaminant intake or dairy-product concentration relative to contaminant intake by food-producing animals

No reported measurements of milk-diet, meat-diet, or egg-diet biotransfer for 2,4-TDI are available in the current literature.

Using guinea pigs exposed to radio-labeled 2,4-TDI in air, Kennedy et al. (1989) have shown that the rate of 2,4-TDI uptake into blood increases linearly with time. They observed a half time for removal of TDI from blood on the order of 400 hours. This observation could be used to establish some preliminary estimate of biotransfer, if it is assumed that half times for removal can be used for other species, that is

$$B_i = \frac{1}{R_b BW} \times \text{or} \pm 50$$

where B_i is the biotransfer factor from animal intake to milk, meat, or eggs, day/kg; R_b is the removal rate constant for 2,4-TDI from the animal, day⁻¹ ($= 0.693/T_{1/2}$); and BW is the animal body weight, kg. The geometric standard deviation accounts for both the uncertainty associated with inter-species extrapolation and the uncertainty associated with relating whole-body blood concentration to concentration in specific tissues. With adult cattle weights in the range 500 to 1000 kg (McKone and Ryan, 1989) and adult chicken weights in the range 1.8 to 2.5 kg (Altman and Dittmer, 1968), we estimate the following uncertain estimates of B_k , B_t , and B_e

$$B_k = 0.032 \text{ d/kg} \times \text{or} \pm 50 \text{ (recommended value for milk)}$$

$$B_t = 0.032 \text{ d/kg} \times \text{or} \pm 50 \text{ (recommended value for meat)}$$

$$B_e = 11 \text{ d/kg} \times \text{or} \pm 50 \text{ (recommended value for eggs)}$$

Contaminant biodegradation factors in soil

Howard et al. (1991) estimate the unacclimated aqueous aerobic biodegradation half life of 2,6-TDI due to aerobic degradation to be in the range of 7 to 28 d. This range corresponds to an aerobic biodegradation rate constant in the range 0.025 to 0.099 d⁻¹. The unacclimated aqueous anaerobic half life for 2,6-TDI has been estimated by Howard et al. (1991) to be in the range of 28 to 112 d. This range corresponds to an anaerobic biodegradation rate constant in the range 0.0057 to 0.025 d⁻¹.

Recommended soil biodegradation rate constants, based on the log mean and log range of the aqueous biodegradation half life ranges above and an uncertainty factor of 2 in going from 2,6- to 2,4-TDI:

aerobic soil biodegradation rate constant = $0.05 \text{ d}^{-1} \times \text{or} + 5$

anaerobic soil biodegradation rate constant = $0.01 \text{ d}^{-1} \times \text{or} + 5$

Media-specific half lives for air, soil, and surface water

- Air* Based on measurements by Atkinson (1987), Howard et al. (1991) estimate the half life of 2,6-TDI in lower atmosphere is in the range of 0.013 to 0.13 d based on photo-oxidation as a removal process.
- Soil* Based on the aqueous hydrolysis half-life in water, Howard et al. (1991) estimate the soil half life of 2,4-TDI to be in the range of 0.5 to 1 d.
- Water* Based on the disappearance due to hydrolysis observed by Duff (1983) of a mixture of 2,4- and 2,6-TDI in a model river, Howard et al. (1991) estimate the half-life of 2,6-TDI in surface water to be in the range 0.5 to 1 d. According to Roegler (1985), the 2,4-isomer is about 1.4 times as reactive with water as the 2,6-isomer.

Recommended half lives (in days), based on geometric mean of the half-lives range and geometric range of the values and an uncertainty factor of 2 in going from 2,6- to 2,4-TDI:

Air $0.04 \times \text{or} + 7 \text{ d}$

Soil $0.7 \times \text{or} + 4 \text{ d}$

Water $0.7 \times \text{or} + 4 \text{ d}$

References for Toluene-2,4-diisocyanate

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1,3-Xylene

Other names: meta xylene, m-xylene, 3-xylene, 1,3-dimethylbenzene, m-xylol

CAS Registry Number: 108-38-3

1,3-xylene is the predominant isomeric form (60%) of the technical grade of xylenes (mixed xylenes) which contains the three isomers and ethylbenzene. Mixed xylenes is produced primarily from petroleum, smaller amounts are produced from coal tar. It is also a by-product of olefin manufacture. Mixed xylenes are ranked 22nd in production volume of top commercial products. Approximately 92% of all mixed xylenes are incorporated into gasoline. The remainder is used in solvent, cleaning agent, and degreaser applications. Individual isomers are used to produce specific industrial chemicals. m-xylene is used for the production of isophthalic acid which is an intermediate in the manufacture of polyester resins. Environmental fate and distribution of mixed xylenes is estimated to be 99.1% through its release into the air from the gasoline fuel emission and solvent waste.

Formula:: C_8H_{10} or $C_6H_4(CH_3)_2$

Molecular weight

106.16 (Windholz et al., 1983)

106.17 (Weast et al., 1986; Howard et al., 1990)

106.2 (Mackay et al., 1992)

Recommended molecular weight for m-xylene, 106.2
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Melting point

-47.4 (Howard et al., 1990)

Octanol-water partition coefficient (K_{ow})

- 1.51 $\times 10^3$ derived from a log K_{ow} of 3.18 reported by Mackay et al. (1992) based on the value measured using generator-column techniques by Wasik et al. (1981).
- 1.95 $\times 10^3$ derived from a log K_{ow} of 3.29 reported by Mackay et al. (1992) based on the value measured using HPLC-k' by Hammers et al. (1982).
- 1.35 $\times 10^3$ derived from a log K_{ow} of 3.13 reported by Mackay et al. 1992) based on the value measured using generator-column, HPLC/UV by Tewari et al. (1982a,b).
- 1.91 $\times 10^3$ derived from a log K_{ow} of 3.28 reported by Mackay et al. (1992) based on the value measured using HPLC/RV by Garst and Wilson (1984).
- 1.58 $\times 10^3$ derived from a log K_{ow} of 3.20 reported by Mackay et al. (1992) based on the value measured using generator-column-HPLC/UV by Wasik et al. (1983).
- 2.34 $\times 10^3$ derived from a log K_{ow} of 3.37 reported by Mackay et al. (1992) based on the value measured using HPLC-k' by Haky and Young (1984).
- 1.51 $\times 10^3$ derived from a log K_{ow} of 3.18 reported by Mackay et al. (1992) based on the value measured by Doucette and Andren (1988).

Recommended value based on the log-mean value of the seven measured values reported above:

$$\log K_{ow} = 3.23 \pm 0.08$$

$$K_{ow} = 1.7 \times 10^3 \times \text{or} \div 1.2$$

Vapor pressure in kPa at standard temperatures

Stull (1947) reports the boiling point of m-xylene as 139.1 °C.

Verschueren (1983) reports the boiling point of m-xylene as 139 °C.

Howard et al. (1990) reports the boiling point of m-xylene as 139.3 °C.

Stull (1947) reports the following vapor pressures for m-xylene.

Temperature (°C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
-6.9	1	0.13
16.8	5	0.67
28.3	10	1.3
41.1	20	2.7
55.3	40	5.3
64.4	60	8.0

Interpolating from these data gives VP at 25 °C = 1.08 kPa

Verschuieren (1983) reports the following vapor pressures for m-xylene.

Temperature (C)	Vapor Pressure (mm)	Vapor Pressure (kPa)
20	6	8.0
30	11	1.5
139	760	101

Interpolating from these data give VP at 25 °C = 1.09 kPa

Other reported values:

- 1.10 reported at 25 °C by Mackay et al. (1982), [Also cited in Mackay et al. (1992)].
- 1.11 reported at 25 °C by Riddick et al. (1986). [Also cited in Mackay et al. (1992) and Howard et al. (1990)].
- 1.11 extrapolated by Mackay et al. (1992) at 25° C from the Antoine equation of Stephenson and Malanowski (1987).
- 1.11 quoted at 25 °C by Hine and Mookerjee (1975). [Also cited in Mackay et al.(1992)].

The following Antoine equations have been published for estimating the vapor pressure of m-xylene in kPa:

$$\log_{10} (\text{VP}) = 6.4629 - \frac{1641.63}{230.9 + T} \pm 0.006 \text{ kPa}$$

for $0\text{ }^{\circ}\text{C} < T < 60\text{ }^{\circ}\text{C}$ from Pitzer and Scott (1943) and cited in Boublik et al. (1984) that gives $VP = 1.12\text{ kPa}$ at $25\text{ }^{\circ}\text{C}$,

$$\log_{10}(VP) = 6.1339 - \frac{1462.27}{215.11 + T} \text{ kPa}$$

for $28\text{ }^{\circ}\text{C} < T < 166\text{ }^{\circ}\text{C}$ from Wilhoit and Zwolinski (1971) and Dean (1985) that gives $VP = 1.11\text{ kPa}$ at $25\text{ }^{\circ}\text{C}$.

The Antoine equation above proposed by Pitzer and Scott (1943) for VP versus temperature is plotted below.

Recommended values for the temperature range $0\text{ to }60\text{ }^{\circ}\text{C}$, based on the Antoine equation of Pitzer and Scott (1943) above:

$$VP(\text{kPa}) = 10^{[6.4629 - 1641.63/(230.9 + T)]} \pm 1 \text{ for } 0\text{ }^{\circ}\text{C} < T < 60\text{ }^{\circ}\text{C}$$

Recommended value @ $25\text{ }^{\circ}\text{C}$, based all values above:

$$VP(\text{kPa}) = 1.10 \pm 0.013 \text{ @ } 25\text{ }^{\circ}\text{C}$$

Solubility in water

- 134 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-GC by Price (1976).
- 146 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-GC by Sutton and Calder (1975).
- 146 mg/L at 25 °C reported by Mackay et al. (1992) based on the value reported by Riddick et al. (1986).
- 157 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-GC by Hermann (1972).
- 159 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using generator column-HPLC/UV by Tewari et al. (1982a).
- 160 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake generator column-HPLC by Wasik et al. (1983), as cited by Shiu et al. (1990).
- 162 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-GC by Polak and Lu (1973).
- 173 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-UV by Andrews and Keefer (1949).
- 196 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-UV by Bohon and Claussen (1951).
- 206 mg/L at 25 °C reported by Mackay et al. (1992) based on the value measured using shake flask-UV by Vesala (1974).

Recommended value based on the arithmetic mean of the ten measured values above:

$$WS = 164 \pm 22 \text{ mg/L @ } 25 \text{ }^{\circ}\text{C}$$

$$= 1.55 \pm 0.21 \text{ mol/m}^3 \text{ @ } 25 \text{ }^{\circ}\text{C}$$

Henry's law constant (dimensionless form, i.e. H/RT)

- 0.26 reported at 25 °C by Nirmalakhandan and Speece (1988). [Also cited in Mackay et al. (1992)].
- 0.29 reported at 25 °C by Pankow and Rosen (1988). [Also cited in Mackay et al. (1992)].
- 0.31 reported at 25 °C by Ashworth et al. (1988). [Also cited in Mackay et al. (1992)]. This value is also reported in Howard et al. (1990) who attributes it to National Academy of Sciences (NAS, 1980) report.
- 0.286 obtained by taking the ratio of VP/WS divided by RT , where VP and WS are the values recommended above.

Recommended value based on the arithmetic mean of the four values above:

$$H/RT = 0.29 \pm 0.02 @ 25\text{ }^{\circ}\text{C}$$

The figure below is the plot of the dimensionless Henry's law constant based on the ratio of temperature-dependent vapor pressure to solubility as recommended in sections above

Organic-carbon partition coefficient (K_{oc})

- 1.82×10^2 derived from a log K_{oc} of 2.26 measured by Seip et al. (1986). [also cited by Mackay et al. (1992)].
- 2.51×10^2 derived from a log K_{oc} of 2.40 measured by Szabo et al. (1990a,b) by using RP-HPLC on two immobilized humic acid phases. [Also cited by Mackay et al. (1992)].
- 2.34×10^2 derived from a log K_{oc} of 2.37 measured by Szabo et al. (1990a,b) by using RP-HPLC on two immobilized humic acid phases. [Also cited by Mackay et al. (1992)].

Recommended value, based on the log-mean value of the three values reported above:

$$\log K_{oc} = 2.34 \pm 0.07$$

$$K_{oc} = 2.20 \times 10^2 \times \text{or} \pm 1.18$$

Diffusion coefficient in water

Based on the Wilke and Chang (1955) method described in Reid et al. (1987), the diffusion coefficient in m^2/d in water is given by

$$D_{xy} = \frac{6.5 \times 10^{-7} (\phi M_y)^{1/2} T}{\eta_y V_x^{0.6}}$$

The molecular weight M_y of water is 18 g/mol. Wilke and Chang (1955) recommend an association factor, ϕ , of 2.6 when the solvent is water. The viscosity of water, η_y , is 0.89 cP at 25 °C. Molecular volume can be estimated by the LeBas incremental method as described in Lyman et al. (1990). With the molecular volume V_x of m-xylene equal to 123 cm^3/mol , this expression gives

Recommended value:

$$D_{\text{water}} = 2.8 \times 10^{-7} T \text{ m}^2/\text{d} = 8.3 \times 10^{-5} \text{ m}^2/\text{d} \text{ or } 9.7 \times 10^{-10} \text{ m}^2/\text{s} @ 25 \text{ }^\circ\text{C}$$

Diffusion coefficient in air

Based on the Fuller et al. (1966) method described in Lyman et al. (1990), the diffusion coefficient in m^2/d in air is given by

$$D_{\text{air}} = 8.6 \times 10^{-3} T^{1.75} \frac{\sqrt{\frac{(29 + M_x)}{29 M_x}}}{\left[2.7 + (V_x)^{1/3}\right]^2}$$

With the molecular volume, V_x , of m-xylene of $123 \text{ cm}^3/\text{mol}$ and a molecular weight of 106.2 g/mol , the above expression gives (with T in kelvins)

Recommended value:

$$D_{\text{air}} = 3.1 \times 10^{-5} T^{1.75} \text{ m}^2/\text{d} = 0.65 \text{ m}^2/\text{d} \text{ or } 7.6 \times 10^{-6} \text{ m}^2/\text{s} @ 25^\circ \text{C}$$

Bioconcentration factors for plant root concentration relative to soil concentration

No reported measurements of plant-root bioconcentration for m-xylene in soils are available in the current literature. Estimation methods for this parameter are considered below.

The partition factor from surface soil to edible plant parts due to rainsplash, $K_{\text{ps}}^{\text{rain}}$ is equal to $0.0034 \text{ kg(soil)/kg(plant)}$ with a CV of 1 (Dreicer et al. 1984). This partition factor applies plant fresh mass concentration relative to soil concentration.

Based on the Briggs et al. (1982, 1983) estimation equation for uptake of contaminants by roots from soil solution, we calculate the RCF (which represents the ratio of contaminant concentration in root, mg/kg [fresh mass], to contaminant concentration in soil solution, mg/L) for m-xylene as

$$\text{RCF} = 10$$

When this factor is divided by the sorption coefficient, $K_D = f_{\text{oc}} \times K_{\text{oc}} = (0.01 \text{ to } 0.02) \times K_{\text{oc}}$ (from above), we obtain the ratio of contaminant concentration in roots, mg/kg (fresh mass) to contaminant concentration in soil solids, mg/kg , which we refer to as $K_{\text{ps}}(\text{roots})$ and estimate it as being in the range

$$K_{\text{ps}}(\text{roots}) = 2.3 \text{ to } 4.5$$

Based the regression of $K_{ps}(\text{roots})$ with K_{oc} from Topp et al. (1986), and based on the range of K_{oc} values listed above, we obtain

(recommended range for root crops)

$$K_{ps}(\text{roots}) = 664 K_{oc}^{-0.622} = 22 \text{ to } 26 \text{ (reflecting the range in } K_{oc}\text{)}$$

Based on the Travis and Arms (1988) correlation for plant-soil bioconcentration we obtain for total plant (not just roots) the following soil/plant partition coefficient

$$K_{ps} = 7.7 K_{ow}^{-0.58} = 0.51 \times \text{or} + 5.3 \text{ (recommended value for exposed produce reflecting estimation error)}$$

Steady-state bioconcentration factors for plant leaf concentration relative to air concentration

No reported measurements of plant-air bioconcentration for m-xylene in air are available in the current literature. Estimation methods for this parameter are considered below.

Based on the model of Riederer (1990) for foliar uptake of gases in plant leaves, we estimate a steady-state plant-air partition coefficient of

$$K_{pa}^{gs} = \left[0.5 + (0.4 + 0.01 \times K_{ow}) \times \frac{RT}{H} \right] \times 10^{-3} \frac{\text{m}^3}{\text{kg}} = 0.06 \text{ m}^3/\text{kg}$$

(recommended value).

We could find no study in which the estimation error of this partition coefficient has been considered, but we assume the CV associated with it is on the order of 1.

Bioconcentration factors for fish concentration relative to water/or sediment concentrations

- 23.44 derived from an eel/water (50 ppm) log BCF of 1.37 reported by Ogata and Miyake (1978).
- 15.14 derived from a goldfish/water log BCF of 1.18 reported by Ogata et al. (1984).
- 6.03 derived from a clam tissue/water log BCF of 0.78 reported by Nunes and Benville (1979).

81 Based the K_{ow} value and the correlation of Mackay (1982).

Recommended value, based on the log-mean value of the three measured values and one predicted value reported above:

$$\log BCF(\text{fish}) = 1.3 \pm 0.5$$

$$BCF(\text{fish}) = 20 \times \text{or} + 3$$

Steady-state biotransfer factors for milk or dairy-product concentration relative to contaminant intake by cattle

No reported measurements of milk-diet biotransfer for m-xylene are available in the current literature.

Based on the geometric mean regression of milk-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the milk biotransfer factor for m-xylene as

$$B_k = 7.9 \times 10^{-9} K_{ow} \times 10^{(\pm 0.84)} = 1.3 \times 10^{-5} \times \text{or} + 7 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CVs of 6.

Steady-state biotransfer factors for meat concentration relative to contaminant intake by cattle, pigs, and chickens

No reported measurements of meat-diet biotransfer for m-xylene are available in the current literature.

Based on the geometric mean regression of meat-to-diet biotransfer against K_{ow} developed by Travis and Arms (1988) we estimate the meat biotransfer factor for m-xylene as

$$B_t = 2.5 \times 10^{-8} K_{ow} \times 10^{(\pm 0.952)} = 4.3 \times 10^{-5} \times \text{or} + 9 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 11.

Steady-state biotransfer factors for egg concentration relative to contaminant intake by chickens

No reported measurements of egg-diet biotransfer for m-xylene are available in the current literature.

Based on the geometric mean regression of egg-to-diet biotransfer against K_{ow} developed above, we estimate the egg biotransfer factor for m-xylene as

$$B_e = 7.9 \times 10^{-6} K_{ow} \times 10^{(\pm 1)} = 1.3 \times 10^{-2} \times \text{or} + 10 \text{ (recommended value)}$$

The estimation error in this expression corresponds to a CV of 14.

Contaminant biodegradation factors in soil

Kappeler and Wuhrmann (1978) report 100% degradation of m-xylene in 192 hours (8 days) in a soil (sampled at 20 and 90 cm depth) column study simulating an *aerobic* ground water infiltration system at 10 °C. This can be interpreted as a residence time and corresponds to a degradation rate of 0.125 day⁻¹.

Jamison et al. (1976) also reported 100% degradation of m-xylene in 192 hours at 13 °C.

Bridie et al. (1979) and Howard et al. (1991) both reported the aqueous, *aerobic* biodegradation half-life of m-xylene in unacclimated soil grab samples in the range 168 to 672 hours (7 to 28 days). [This study is also cited in Mackay et al. (1992)]. This range of soil half-lives corresponds to a soil biodegradation rate constant of 0.099 day⁻¹ to 0.025 day⁻¹.

Kuhn et al. (1985) and Howard et al. (1991) both reported the aqueous, *aerobic* biodegradation half-life of m-xylene in unacclimated soil grab samples from which an aqueous *anaerobic* biodegradation half-life in the range 672 to 2688 hours (28 to 112 days) is derived. [This study is also cited in Mackay et al. (1992)]. This range of soil half-lives corresponds to a soil biodegradation rate constant of 0.025 to 0.00026 day⁻¹.

Olsen and Davis (1990) report a biodegradation half time of 0.7 hours (0.03) days. [This study is also cited in Mackay et al. (1992)]. This half-life corresponds to a soil biodegradation rate constant of 23.1 day⁻¹.

Recommended values, based on log mean of the soil degradation rate constants:

aerobic soil biodegradation rate constant = 0.24 day⁻¹ × or + 12

anaerobic soil biodegradation rate constant = 0.0025 day⁻¹ × or + 4

Media-specific half lives for air, soil, and surface water

Air Atkinson (1985) estimated the half life of m-xylene in the lower atmosphere to be 2.6 to 26 hours (0.1 to 1.1) days based on an measured rate data for vapor phase reacton with hydroxy radicals in air. [Also reported by Howard et al. (1991) and cited by Mackay et al. (1992)].

Singh et al. (1981) estimated the half life of m-xylene in urban lower atmospher to be 7.2 hours (0.3) days based on an measured rate data for vapor phase reacton with hydroxy radicals at 27 °C.

Doyle et al. (1975) estimated the half life of m-xylene in ambient LA basin to be 0.83 hour based on an measured reacton with hydroxy radicals at 27°C. [Also cited by Mackay et al. (1992)].

Brice and Derwent (1978) estimated the half life of m-xylene in the lower atmosphere under smog in S.E. England to be 1.5 hours (0.06) days. [also reported by Perry et al. (1977), and cited by Mackay et al. (1992)].

Ravishankara et al. (1978) estimated the half life of m-xylene in the troposphere to be 1.0 hours (0.042) day for summer and 9.7 hours (0.4) day for winter based on an measured rate data for vapor phase reacton with hydroxy radicals at 25 °C.

Soil Howard et al. (1991) have estimated the half-live of m-xylene in soil due to aerobic biodegradation to be in the range of 168 to 672 hours (7 to 28 days). [also reported by Bridie et al. (1979), and cited by Mackay et al. (1992)].

Water Howard et al. (1991) have estimated the half-live of m-xylene in surface water due to aerobic biodegradation to be in the range of 168 to 672 hours (7 to 28 days).

Recommended half-life values, based on arithmetic mean of the half lives and geometric range of the values:

Air 0.3 d × or ÷ 2.6

Soil 18 d × or ÷ 1.5

Surface Water 18 d × or ÷ 1.5

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