FINAL DRAFT REPORT

Intermedia Transfer Factors for Contaminants Found at Hazardous Waste Sites

1,4-DICHLOROBENZENE
(*p*-DCB)

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The Department of Toxic Substances Control (DTSC), within the California Environmental Protection Agency, has the responsibility for managing the State's hazardous-waste program to protect public health and the environment. The Office of Scientific Affairs (OSA) within the DTSC provides scientific assistance in the areas of toxicology, risk, environmental assessment, training, and guidance to the regional offices within DTSC. Part of this assistance and guidance is the preparation of regulations, scientific standards, guidance documents, and recommended procedures for use by regional staff, local governmental agencies, or responsible parties and their contractors in the characterization and mitigation of hazardous-waste-substances-release sites. The CalTOX model has been developed as a spreadsheet model to assist in exposure and health-risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water.

The modeling effort includes multimedia transport and transformation models, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models. Use of the CalTOX model requires that we determine the intermedia transfer factors (ITFs) that define concentration relationships between an exposure medium and the environmental medium that is the source of the contaminant. ITFs are chemical and physical parameters which serve as inputs in the CalTOX model analysis.

This report provides a set of ITFs needed to run the CalTOX model for p-DCB. For this chemical, we have conducted a critical review of existing literature for measured values and estimation methods in order to compute an arithmetic mean ($\bar{x}$), a coefficient of variation (CV), and plausible range for each ITF.

OVERVIEW

The purpose of this report is to provide a set of chemical-specific intermedia-transfer factors (ITFs) for *p*-DCB. We have carried out a critical review of the existing literature in order to identify a mean value, coefficient of variation (CV) and value range for the ITFs listed in Table 1. For values used to define a given parameter, our highest priority was given to experimental values reported in the primary scientific literature, that is, peer-reviewed journals. For parameters that are not readily available from the primary literature, widely cited secondary references such as Lyman et al. (1982, 1990), Verschueren (1984), Howard et al. (1990, 1991), Mackay et al. (1992), the CRC Handbook (1989-90) and the Merck Index (1983, 1989) are used to establish parameter values. When measured values are not available from either the primary literature or secondary references, estimates of ITF parameter values are based on estimation equations that are available in the primary literature. Typically, these estimation methods relate ITFs to other measured contaminant parameters using quantitative-structure-activity-relationship (QSAR) methods. In these cases, parameter values estimated from a QSAR method are treated as the arithmetic mean and the estimation error of the method is used to determine the CV. Table 1 summarizes the units required by the CalTOX model, the values of chemical specific physico-chemical properties, distribution coefficients, biotransfer and bioconcentration factors, and transformation half-lives obtained in this study.

CalTOX Chemical-Specific Input Requirements

The CalTOX model uses three sets of input data—one describing the chemical-specific properties of the contaminants, a second providing properties of the environment or landscape receiving the contaminants, and a third that defines for exposure assessment the characteristics of individuals in various age/sex categories and the characteristics of the micro-environments in which they live or from which they obtain water and food. Each of the inputs in these sets must be described in terms of a mean value with an estimated coefficient of variation, which describes the uncertainty or variability associated with that parameter. This report addresses mean value, CV, and range of values needed to characterize chemical-specific inputs.

Physicochemical Properties

Physicochemical properties include molecular weight, octanol-water partition coefficient, melting point, vapor pressure, Henry's law constant, diffusion coefficients in air and water, and the organic-carbon partition coefficient. The octanol-water partition coefficient provides a measure of the extent of chemical partitioning between water and octanol at equilibrium and is used as a basis for estimating other ITF parameters. The melting point is the temperature at which a compound makes the transition from a solid to a liquid phase. Vapor pressure is the pressure exerted by a chemical vapor in equilibrium with its solid or liquid phase. Water solubility is the upper limit on a chemical's dissolved concentration in pure water, at a specified temperature.

Table 1. Summary of Chemical Properties for 1,4-Dichlorobenzene

Description	Symbol	Mean Value	Coefficient of Variation	Number of Values
Molecular Weight (g/mol)	MW	147	2.5×10^{-5}	5
Octanol-Water Partition Coefficient	K_{ow}	3100	0.39	10
Melting Point (K)	T_m	326.3	8.1×10^{-4}	5
Vapor Pressure (Pa)	VP	150	0.44	5
Solubility (mol/m^3)	S	0.51	0.23	10
Henry's Law Constant (Pa-m^3/mol)	H -	260	0.20	4
Diffusion Coefficient in Pure Air (m^2/d)	D_{air}	0.61	0.08	e
Diffusion Coefficient in Pure Water (m^2/d)	D_{water}	7.8×10^{-5}	0.25	e
Organic Carbon Partition Coefficient	K_{oc} -	570	0.76	8
Distribution Coefficient in Ground-Surface and Root-Zone Soil	K_{d_s} -	b	e	e
Distribution Coefficient in Vadose-Zone Soil	K_{d_v} -	b	e	e
Distribution Coefficient in the Ground-Water Zone	K_{d_q} -	b	e	e
Distribution Coefficient in Ground Water Sediment	K_{d_d} -	b	e	e
Partition Coefficient in Plants Relative to Soil Concentration [ppm (pFM) /ppm (sFM)]	K_{ps} -	0.37	0.48	2
Biotransfer Factor in Plants Relative to Contaminant Air Concentration [m^3(a)/kg (pFM)]	K_{pa} -	0.29	14	e
Biotransfer Factor in Milk Relative to Cattle-Diet Contaminant Intake (d/kg)	B_k -	1.7×10^{-5}	11	e
Biotransfer Factor in Meat Relative to Cattle-Diet Contaminant Intake (d/kg)	B_t -	1.0×10^{-4}	13	e
Biotransfer Factor in Eggs Relative to Hen-Diet Contaminant Intake (d/kg)	B_e -	0.024	14	e
Biotransfer in Breast Milk Relative to Contaminant Intake by the Mother (d/kg)	B_{bmk} -	6.2×10^{-4}	10	e
Bioconcentration Factor in Fish Relative to Contaminant Water Concentration	BCF -	290	0.90	14
Skin Permeability Coefficient (cm/h)	K_{p_w} -	0.11	2.4	e
Skin-Water/Soil Partition Coefficient [ppm (skin)/ppm (water)]	K_m -	150	0.27	e
Reaction Half-Life in Air (d)	T_{half_a}	38	1.5	2
Reaction Half-Life in Ground-Surface Soil (d)	T_{half_g}	520	0.53	5
Reaction Half-Life in Root-Zone Soil (d)	T_{half_s}	520	0.53	5
Reaction Half-Life in the Vadose-Zone Soil (d)	T_{half_v}	520	0.53	5
Reaction Half-Life in Ground-Water Zone Soil (d)	T_{half_q}	450	1.7	3
Reaction Half-Life in Surface Water (d)	T_{half_w}	12	1.1	5
Reaction Half-Life in the Sediment (d)	T_{half_d}	180	1.7	5

[a]Values followed by a "-" include default equations that can be used for estimations
[b]$K_d = [(K_{oc}) \times$ (fraction organic matter)], a site and soil zone specific parameter
[e]estimated parameter value

Henry's law constant is a measure at equilibrium of the ratio of chemical activity in the gas above a liquid to chemical activity in the liquid. Diffusion coefficients describe the movement of a molecule in a liquid or gas medium as a result of differences in concentration within the medium. 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. The organic-carbon partition coefficient provides a measure of chemical partitioning between organic carbon (in soils, rocks, 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.

The Solid-Water Distribution Coefficients

The distribution or sorption coefficient, K_d, is the concentration ratio, at equilibrium, of chemical attached to solids and/or particles (mol/kg) to chemical concentration in the solution, mol/L. 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. CalTOX requires, as input, distribution coefficients for ground-surface, root-zone, and vadose-zone soil; ground-water-zone rock or soil, and surface-water sediments.

Biotransfer Factors and Bioconcentration Factors

The CalTOX model requires, as input, general relationships that can be used to estimate partition coefficients between air and plants; between soil and plants; between animal feed intake and animal-based food products; between surface water and fish; between the human mother's uptake and breast milk; between skin and water; and between skin uptake and concentration in skin water.

The chemical-specific plant-air partition coefficient, K_{pa}, represents the ratio of contaminant concentration in above-ground plant parts, in mg/kg (fresh mass), to contaminant concentration in the gas-phase of the atmosphere mg/m^3 (air). The plant-soil partition coefficient, K_{ps}, expresses the ratio of contaminant concentration in plant parts, both pasture and food, in mg/kg (plant fresh mass) to concentration in wet root-zone soil, in mg/kg.

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. These factors 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.

Lactating women can transfer to breast milk their intake of contaminants from all intake routes—ingestion, inhalation, and dermal contact. B_{bmk} is the biotransfer factor for milk-concentration versus the mother's intake. This relationship may also be described as the ratio of contaminant concentration in mother's milk divided by the mother's daily intake of that contaminant, in units of d/kg (milk).

The bioconcentration factor BCF provides a measure of chemical partitioning between fish tissue based on chemical concentration in water.

Chemical specific exposure factors used in CalTOX include the skin-water and skin-soil partition coefficients. K_m is the skin-water partition coefficient in cm^3 (water)/cm^3 (skin) . In order to estimate the skin-soil partition factor, K_m^{soil}, with units cm^3 (soil)/cm^3 (skin), we divide equation K_m by the sorption coefficient K_d for soil, or

$$K_m^{soil} = \frac{K_m}{K_d}$$

K_{p_w} is the steady-state permeability coefficient in cm/hour for a contaminant from water on skin through stratum corneum and can either be based on a measured value or estimated values.

Chemical-Specific Transformation Process Half-Lives

Chemical transformations, which may occur as a result of biotic or abiotic processes, can have a profound effect on the persistence of contaminants in the environment. Experimental methods and estimation methods are available for defining these fate processes in a variety of media. Specific information on the rates and pathways of transformation for individual chemicals of concern should be obtained directly from experimental determinations, if possible, or derived indirectly from information on chemicals that are structurally similar. CalTOX makes use of media- and reaction-specific reaction half-lives to establish rate constants for transformation removal processes that include photolysis, hydrolysis, oxidation/reduction, and microbial degradation.

Transformation-rate half-lives are among the more uncertain parameters in the CalTOX model. There are typically few available measurements or ranges of estimated values in the primary and secondary literature. Most of the available half-life values are obtained from limited measurements for environmental media that are not necessarily representative of those in California. These values often involve scientific judgment as much as measurement. In making use of these data, we expanded the range of the reported values by a factor of 5 when only 2 or 3 representative values are presented and by a factor of 10 when only one value is provided. If 4 or more measured values are available, these uncertainty factors are not applied. In order to express the lack of reliability associated with a limited number of measured values for a parameter, these uncertainty factors are used to express both large uncertainty and significant variability.

Statistical Methods

Each of the inputs to CalTOX must be described by a mean value and an estimated coefficient of variation which describes the uncertainty or variability associated with

that parameter. For input values that are derived from a number of measured values, the mean and coefficient of variation are obtained from the arithmetic mean and the arithmetic standard deviation of the inputs. For estimated input values, the mean and coefficient of variation are obtained from an estimation equation and the residual error of the estimation equation. The methods we used to obtain these values are described here.

Mean and Coefficient of Variation

The arithmetic mean ($\bar{x}$) is used to represent all inputs that are derived from a number of measured values—even those that might have geometric distributions. The ($\bar{x}$) is computed by summing the reported values and dividing this sum by the total number of observations:

$$Arithmetic\ mean\ (\mathbf{\bar{x}}) = \frac{\sum_{i=1}^{n} \mathbf{x_i}}{\mathbf{n}} \qquad (Eqn.\ 1)$$

Where $\sum_{i=1}^{n} \mathbf{x_i}$ is the sum of the observed values and n is the number of observations. In this case, the coefficient of variation (CV) is computed by dividing the arithmetic standard deviation ($\mathbf{s_n}$) by the mean. Standard deviation and CV are computed according to the following equations:

$$standard\ deviation\ (\mathbf{S_n}) = \frac{\sum_{i=1}^{n} (\mathbf{x_i} - \mathbf{\bar{x}})^2}{\mathbf{n}} \qquad (Eqn.\ 2)$$

$$coefficient\ of\ variation\ (\mathbf{CV}) = \frac{\mathbf{S_n}}{\mathbf{\bar{x}}} \qquad (Eqn.\ 3)$$

It should be noted that, based on the central limit theorem of statistics, the confidence associated with the estimate of $\bar{x}$ from above becomes large as the number of samples used to estimate $\bar{x}$ also becomes large. Therefore, the reliability of the estimates of *mean* and *CV* of a parameter are low when the sample size is small. It is beyond the scope of this document to explicitly address the reliability of these estimates. Nonetheless, in order to give an indication of potential reliability problems, we list the number of measurements used to estimate the mean and CV of each parameter in the last column of Table 1.

Estimation Equations and the Residual Errors of the Estimation Method

Estimates of some CalTOX inputs are based on regression equations that relate a parameter value to some measure of structure or activity associated with the contaminant. These methods are referred to as quantitative structure-activity

relationship (QSAR) methods. The reliability of a parameter-value estimated in this way is defined by the precision of these QSAR methods.

Our estimate of precision in QSAR estimation methods is based on calculating, S_e, the *standard error of the estimate* (or standard deviation of the residuals). This error calculation is based on the regression equations and fragment models used to derive a parameter value. To illustrate, when the value of parameter such as the organic-carbon partition coefficient (K_{oc}) is estimated using a regression or correlation analysis, the S_e is calculated using the following approach (Hamburg, 1970). First, since it is typical that it is the $\log K_{oc}$ (not K_{oc} itself) that is estimated from a regression equation, we calculate the S_e of $\log K_{oc}$ according to

$$S_e \text{ of } \log K_{oc}^{est} = \frac{\sum_{i=1}^{n} (\log K_{oc}^{msd} - \log K_{oc}^{est})^2}{(n-2)} \qquad \text{(Eqn. 4)}$$

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. In order to calculate the S_e of K_{oc}, we make use of the transformation

$$GSD (K_{oc}^{est}) = 10^{(S_e \text{ of } \log K_{oc}^{est})} \qquad \text{(Eqn. 5)}$$

to calculate the geometric standard deviation of S_e (GSD) of K_{oc}^{est}, which is simply the GSD of the K_{oc} estimate, that is GSD (K_{oc}^{est}). It has been shown by Atchison and Brown (1957) that the relationships between the GSD and CV for log normal distributions are as follows

$$GSD = \exp\left\{ \ln(1+CV^2) \right\} \qquad \text{(Eqn. 6)}$$

$$CV = \left(\exp\left\{ [\ln(GSD)]^2 \right\} - 1 \right) \qquad \text{(Eqn. 7)}$$

Since the implicit assumption of a regression for estimating the log of K_{oc} is that any estimated value, $\log (K_{oc}^{est})$, is centered on normal distribution with standard deviation equal to S_e of $\log K_{oc}$, it follows that the corresponding estimated value of K_{oc} is centered on a log normal distribution with GSD (K_{oc}^{est}) and with

$$CV\ (K_{oc}^{est}) = \exp\left\{[\ln(GSD(K_{oc}^{est}))]^2\right\} - 1 \qquad \text{(Eqn. 8)}$$

This approach is used to estimate CVs for the estimation equations presented in this document.

In some cases the error term, CV for example, is calculated by combining through the operations of multiplication and division the CVs of two or more parameters. For example the CV in the ration H = VP/S is combined from the CV (VP) and CV (S). In this case, if the input parameters are independent, the combined CV is calculated using the following equation:

$$CV_{combined} = \frac{\sum_{i=1}^{n} CV_i^2}{n} \qquad \text{(Eqn. 9)}$$

where n is the number of parameters used in the multiplication/division and CV_i is the coefficient of variation in the ith input parameter.

1,4 Dichlorobenzene

Other Names

1,4-dichlorobenzene; *p*-Dichlorobenzene; paradichlorbenzene; para-Chlorophenyl chloride; PDB; PDCB; Chemical Abstracts Services Registration Number: 106-46-7 (WHO IARC 1982); *p*-Chlorophenyl Chloride; Di-Chloricide; *p*-Dichlorobenzol; Dichlorobenzene; PARA solid (DOT); EVOLA; NCI-C54995; Paracide; Para Crystals; Paradi; Paradichlorobenzene; Paradichlorozenzol: Paradow; Paramoth; Paranuggets; Parazzene; Persia-Perazol; RCRA Waste Number U070, UO71, U072; Santochlor (Sax and Lewis, 1989)

Background

1,4-dichlorobenzene (*p*-DCB) is produced commercially by the direct chlorination of benzene in the liquid phase. Approximately 30-50% of *p*-DCB produced has been used as a space deodorant for toilets and refuse containers or as a fumigant for moths, molds, and mildews. A significant amount of *p*-DCB is used in the production of PPS resins and as an intermediate for production of other chemicals. Minor use of *p*-DCB includes its use as a solvent for various applications such as paint, gums, etc. Detection of *p*-DCB in groundwater indicates that leaching can occur, though analysis of data in the Great Lakes area shows that binding to soil and sediment is a fate process affecting large amounts of *p*-DCB [Howard (1991)]. When released to water, volatilization is expected to be the major removal process. An estimated 70-90% of the annual US production of *p*-DCB is reported to be released into the air at a relatively rapid rate. *p*-DCB is also reported to be reactive toward hydroxyl radicals in air [ATSDR (1989)].

Formula

$C_6 H_4 Cl_2$
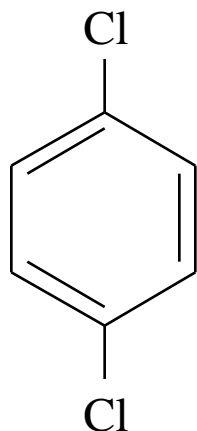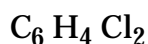
MW: Molecular Weight

The units used for molecular weight are grams/mole (g/mol).

Reported Values

147	reported as 147 g/mol in CRC Handbook [Weast et al. (1989)]
147.003	reported as 147.003 g/mol by Daubert and Danner (1985)
147.004	reported as 147.004 g/mol by Daubert and Danner (1989)
147.005	reported as 147.005 g/mol by Kirk-Othmer (1985)
147.01	reported as 147.01 g/mol by Mackay et al. (1992)

> From the above 5 reported values above, we obtain the following statistics for the molecular weight of p-DCB:
>
> Arithmetic mean (coefficient of variation):
> MW = 147 (2.5×10^{-5}) g/mol

Range: 147 to 147.01

K_{ow}: Octanol-Water Partition Coefficient

The units used for K_{ow} are $\dfrac{\text{mg/liter (octanol)}}{\text{mg/liter (water)}}$ and K_{ow} is therefore unitless.

Experimental Values

2344	reported at 20 °C as a log K_{ow} of 3.37 by Veith et al. (1980) using a shake-flask method
2399	reported at 20 °C as a log K_{ow} of 3.38 by Freed et al. (1979) using a shake-flask GC method
6026	reported at 20 °C as a log K_{ow} of 3.78 by Veith et al. (1980) estimated using RP-HPLC
4169	reported at 22 °C as a log P of 3.62 by Konemann (1979) using a shake flask-HPLC method
2340	reported at 23 °C as a K_{ow} of 2340 by Banerjee et al. (1980) using a shake flask-LSC
2344	reported at 25 °C as a log K_{ow} of 3.37 by Wasik (1981) estimated using a generator column-HPLC method
2399	reported at 25 °C as a log K_{ow} of 3.38 by Miller et al. (1984) estimated using a modified generator column coupled with a HPLC (GC-HPLC)
2692	reported at 25 °C as a log K_{ow} of 3.43 by Hammers et al. (1982) estimated using a value measured by Reverse Phase High Performance Liquid Chromatography (RP-HPLC) [Also cited in Mackay et al. (1992)]

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2780   reported at 25 °C as a log K_{ow} of 3.444 by De Bruijn et al. (1989) using a slow-stirring method

3290   reported at 25 °C as a K_{ow} of 3290 by Wataral (1982) using a shake flask-GLC method

From the 10 measured values above we obtain the following statistics for the octanol-water partition coefficient of *p*-DCB at 20 to 25 °C:

Arithmetic mean (coefficient of variation):
K_{ow} = 3100 (0.39)

Range: 2340 to 3290

Other Values

3631   reported at an indeterminate temperature as a log K_{ow} of 3.56 by Periera et al. (1988) using saline water (0.8%) and a shake-flask GC method

T_m: Melting Point

The units used for melting point are kelvins (K).

Reported Values

325.99   reported as a MP of 52.84 °C by Gross and Saylor (1931)

326.14   reported as a FP of 52.99 °C by McDonald et al. (1959) [also cited in Riddick et al. (1986)]

326.25   reported as a MP of 53.1 °C by Yalkowsky and Valvani (1980)

326.28   reported as a FP of 53.13 °C by Walsh and Smith (1961)

326.7   reported as a MP of 326.7 K by Miller et al. (1984)

From the 5 measured values above, we obtain the following statistics for the melting point of *p*-DCB:

Arithmetic mean (coefficient of variation):
T_m = 326.3 (8.1 × 10^{-4}) K

Range: 325.99 to 326.7 K

Other Values

326.14   reported as a MP of 326.14 K by Stull (1947)

326.15   reported as a MP of 53 °C Clayton and Clayton [Patty's Industrial Hygiene and Toxicology (1981)]

326.25   reported as a MP of 53.1 °C in the CRC Handbook [Weast et al. (1989)]

VP: Vapor Pressure at Standard Temperatures

The units used for vapor pressure are pascals (Pa).

Reported Values

86.7	reported at 20 °C as a saturation vapor pressure of 0.65 mm Hg by Chiou & Shoup (1985) using a chemical vapor generator-GC method
121	reported at 23.9 °C as 0.91 mm Hg by Walsh and Smith (1961) using a sulfuric acid manometer and temperatures 20.4 < T < 52.5 °C
135	extrapolated to 25 °C corresponding to 1.01 mm Hg by Darkis et al. (1940) using 5 < T < 30 °C
143	extrapolated to 25 °C corresponding to 143 Pa by Verscheuren et al. (1983) and Weast et al. (CRC Handbook, 1986) using 20 < T < 84.8 °C
260	extrapolated to 25 °C corresponding to 260 Pa by Stull (1947) using 54.8 < T < 95.2 °C

> From the 5 measured values above, we obtain the following statistics for the vapor pressure of p-DCB at 20-25 °C:
>
> Arithmetic mean (coefficient of variation):
>   VP = 150 (0.44) Pa

Range: 86.7 to 260 Pa

Estimation Methods

The following Antoine equations have been published for estimating the vapor pressure of p-DCB in kPa

Antoine Equation 1

The following Antoine equation is reported by Stull (1947).

$$\log_{10} \text{VP (Pa)} = 10.2385498 - \frac{2331.41449}{273 + \text{T (°C)}}$$

using 54.8 < T < 95.2 °C, yielding:

VP = 260 Pa at 25 °C

<u>Antoine Equation 2</u>

The following Antoine equation is derived from data reported by Walsh and Smith (1961).

$$\log_{10} VP \ (Pa) = 13.181756 - \frac{3292.5574}{273 + T \ (°C)}$$

for 20.4 °C < T < 36.4 °C, yielding:

VP = 135 Pa at 25 °C

<u>Antoine Equation 3</u>

The following Antoine equation is derived from data reported by Darkis et al. (1940).

$$\log_{10} VP \ (Pa) = 11.985 - \frac{3570}{273 + T \ (°C)}$$

for 5 < T < 30 °C, yielding:

VP = 135 Pa at 25 °C

S: Solubility in Water

The units used in the solubility values below are $\frac{mg}{liter \ (water)}$ (mg/L).

Experimental Values

83.4	reported at 24.6 °C as 83.4 mg/L by Wauchope and Getzen (1972) using a shake flask-UV method
30.9	reported at 25 °C as 2.10×10^{-4} mol/L by Miller et al. (1984) using a modified generator column coupled with a HPLC
65.3	reported at 25 °C as 65.3 mg/L by Banerjee (1984) using shake flask-HPLC
73.7	reported at 25 °C as a log 1/Solubility of 3.30 mol/L by Veith et al. (1980) using a shake flask-LSC method
73.8	reported at 25 °C as 502 μM by Banerjee et al. (1980) using a shake-flask method [also cited in Horvath (1982)]
76	reported at 25 °C as 0.0076 g/100 cc by Andrews (1950) using a shake flask-UV method
79	reported at 25 °C as 79 ppm in water by Freed et al. (1979) using a stir flask-GLC method

85   reported at 25 °C as as 0.58×10^{-6} mol/g water by Vesala (1974) using a shake flask-UV method

87.15   reported at 25 °C as 87.15 mg/L by Aquan-Yuen et al. (1979)

90.6   reported at 25 °C as a log Sol of -3.21 mol/L by Yalkowsky and Valvani (1980) by a shake flask-UV method

Unit Conversion

Arithmetic mean (coefficient of variation) of *p*-DCB solubility

= 74.5 (0.23) mg/L

= 0.51 (0.23) mol/m^3

From the 10 measured values above, we obtain the following statistics for the water solubility of *p*-DCB at 25 °C:

Arithmetic mean (coefficient of variation):
    S = 0.51 (0.23) mol/m^3

Range: 0.21 to 0.62 mol/m^3

H: Henry's Law Constant

The units used for Henry's Law constant are $\dfrac{\text{Pascals-m}^3}{\text{mole}}$ (Pa-m^3/mol).

Experimental Values

193   reported at 20 °C as 0.078 unitless by Yurteri et al. (1987) using Equilibrium Partitioning in Closed Systems (EPICS)

262   reported at 20 °C as 0.00259 atm-m^3/mol by Ashworth et al. (1988) measured by EPICS [Also cited in Mackay et al. (1992)]

276   reported at 25 °C as 0.00272 atm-m^3/mol by Warner et al. (1987) using a modified batch stripping apparatus

321   reported at 25 °C as 0.00317 atm-m^3/mol by Ashworth et al. (1988) measured by EPICS [Also cited in Mackay et al. (1992)]

From the 4 measured values above, we obtain the following statistics for Henry's law constant at 20-25 °C:

Arithmetic mean (coefficient of variation):
    H = 260 (0.20) Pa-m^3/mol

Range: 193 to 321 Pa-m^3/mol

Estimation Method

$$H = \frac{VP\ (Pa)}{S\ (mol/m^3)} = \frac{150}{51} = 290\ (0.47)\ Pa\text{-}m^3/mol\ at\ 20\text{-}25\ °C$$

D_{air}: Diffusion Coefficient in Pure Air

The units used for the diffusion coefficient in pure air are $\frac{meters^2}{day}$ (m^2/d).

Estimation Method

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

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

Molar volume (V_x) can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With a molar volume, V_x, of 137.8 cm^3/mol, molecular weight (M_x) of 147 g/mol, and a temperature equal to 298 K, the above expression gives:

$$D_{air} = 2.83 \times 10^{-5}\ T^{1.75} = 0.61\ m^2/d$$

The reported average absolute estimation error is 5 to 10% (Fuller et al., 1966) and is equivalent to the CV reported below.

Based on the estimated value and the estimation error reported above, we obtain the following statistics for the estimated air diffusion coefficient of *p*-DCB at 25 °C:

      Arithmetic mean (coefficient of variation):
            $D_{air} = 0.61\ (0.08)\ m^2/d$

D_{water}: Diffusion Coefficient in Pure Water

The units used for the diffusion coefficient in pure water are $\frac{meters^2}{day}$ (m^2/d).

Estimation Method

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

$$D_{water} = \frac{6.5 \times 10^{-7} \quad f \times M_y\, T}{h_y\, V_x^{0.6}}$$

Wilke and Chang (1955) recommend an association factor, f, of 2.6 when the solvent is water. The viscosity of water, h_y, is 0.89 cP at 25 °C. Molar volume (V_x) can be estimated by the LeBas incremental method as described in Lyman et al. (1982). With a V_x equal to 137.8 cm^3/mol, a temperature (T) of 298 K, and M_y (MW of water) equal to 18 g/mol., this expression gives:

$$D_{water} = 2.6 \times 10^{-7}\, T = 7.8 \times 10^{-5}\ m^2/d\ at\ 25\ °C$$

Original data for this estimation, provided in Reid et al. (1987), can be used to determine the standard error of the estimator for this estimation method. From this data we calculate a CV of 0.25 from a 25% estimation error.

Based on the estimated value and the estimation error reported above, we obtain the following statistics for the estimated water diffusion coefficient of p-DCB at 25 °C:

Arithmetic mean (coefficient of variation):
$D_{water} = 7.8 \times 10^{-5}$ (0.25) m^2/d

K_{oc}: Organic-Carbon Partition Coefficient

The units used for K_{oc} are $\dfrac{\text{mg/kg (organic carbon)}}{\text{mg/kg (water)}}$ and K_{oc} is therefore unitless.

Experimental Values

251	reported as a log K_{oc} of 2.4 by Topp (1986) using soil (f_{oc} = 2.06%, pH = 6.4) for 1 week and ^{14}C labelled p-dichlorobenzene
273	reported at 20 °C as a log K_{om} of 2.2 by Chiou et al. (1983) using a Woodburn silt loam soil with 1.9% organic matter and assuming K_{oc} = $K_{om} \times 1.724$
373	reported as a K_f (soil/water) of 8 by Cornelis et al. (1991) using a sandy soil and an artificial OECD mixture (f_{om} = 3.7%, pH = 4.8)
383	reported as a K_f (soil/water) of 18 by Cornelis et al. (1991) using a sandy soil and an artificial OECD mixture (f_{om} = 8.1%, pH = 5.90)
429	derived from an average K_{om} of 249 by Friesel et al. (1984) and assuming that $K_{oc} = K_{om} \times 1.724$
598	reported as an average K_{oc} of 598 by Southworth and Keller (1986) using 3 soils (f_{oc} = 0.069 to 1.29%; pH = 4.2-4.5)

700　　　　　reported as a K_{oc} of 700 by Hutzler et al. (1983) using 20 soils (0.1 to 12% f_{oc}, 4.1-8.6 pH)

1587　　　　reported at 21 °C as a Freundlich K of 40.5 by Uchrin et al. (1986) using 4.06 and 4.15 mg/L in aquifer solids from a New Jersey aquifer (f_{om} = 4.4%) and assuming $K_{oc} = K_{om} \times 1.724$

From the 8 measured values above, we obtain the following statistics for the organic carbon partition coefficient for p-DCB:

Arithmetic mean (coefficient of variation):
K_{oc} = 570 (0.76)

Range: 251 to 1587

Other Values

79,433　　　reported as a log K_{oc} in sediment of 4.8 and 5.0 by Oliver and Charlton (1984) using field sediment trap material (4.1% organic carbon) and Niagara river organic matter and measured water concentrations from July 1981 (they assume $f_{oc} = 2*f_{om}$)

Estimation Method

Karickhoff (1981) has described empirical estimation methods for obtaining K_{oc} from K_{ow}. The most general of these is that K_{oc} is equal to 0.41 times K_{ow}.

$$K_{oc} = 0.41 \times K_{ow}$$
$$K_{ow} = 3100$$

$$K_{oc} \text{ (est)} = 1300 \text{ (1)}$$

The reported CV is based on data provided by Karickhoff (1981). This estimation error does not include uncertainty in the value of K_{ow}.

K_{d_s}: Distribution Coefficient in Ground-Surface and Root-Zone Soil

The units used for K_{d_s} are $\dfrac{\text{mg/kg (dry surface and root-zone soil)}}{\text{mg/kg (water)}}$ and K_{d_s} is therefore unitless.

Estimation Method

This is a site specific parameter and depends on the fraction organic carbon in the surface and root-zone soil and on the value of K_{oc}. K_{d_s} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction organic carbon in the surface and root-zone soil (f_{oc_s}) (Karickhoff, 1981).

$$K_{d\_s} = K_{oc} \times f_{oc\_s}$$

$$f_{oc\_s} = \frac{\text{kg organic carbon (dry surface and root-zone soil)}}{\text{kg (soil)}}$$

> Based on the estimation reported above, we obtain the following equation for the distribution coefficient in surface and root-zone soil. K_{d_s} is a site and soil-zone specific parameter depending on the fraction organic carbon in the surface and root-zone soil or:
>
> $$K_{d\_s} = K_{oc} \times f_{oc\_s}$$

K_{d_v}: Distribution Coefficient in Vadose-Zone Soil

The units used for K_{d_v} are $\dfrac{\text{mg/kg (dry vadose-zone soil)}}{\text{mg/kg (water)}}$ and K_{d_v} is therefore unitless.

Estimation Method

This is a site specific parameter and depends on the fraction organic carbon in the vadose-zone soil and on the value of K_{oc}. K_{d_v} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction organic carbon in the vadose-zone soil (f_{oc_v}) (Karickhoff, 1981).

$$K_{d\_v} = K_{oc} \times f_{oc\_v}$$

$$f_{oc\_v} = \frac{\text{kg organic carbon (dry vadose-zone soil)}}{\text{kg (soil)}}$$

> Based on the estimation reported above, we obtain the following equation for the distribution coefficient in vadose-zone soil. K_{d_v} is a site and soil-zone specific parameter depending on the fraction organic carbon in the vadose-zone or:
>
> $$K_{d\_v} = K_{oc} \times f_{oc\_v}$$

K_{d_q}: Distribution Coefficient in the Ground-Water Zone

The units used for K_{d_q} are $\dfrac{\text{mg/kg (dry aquifer material)}}{\text{mg/kg (water)}}$ and K_{d_q} is therefore unitless.

Estimation Method

This is a site-specific parameter and depends on the fraction organic carbon in the ground-water zone and on the value of K_{oc}. K_{d_q} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction organic carbon in the ground-water zone (f_{oc_q}) (Karickhoff, 1981).

$$K_{d\_q} = K_{oc} \times f_{oc\_q}$$

$$f_{oc\_q} = \frac{\text{kg organic carbon (dry aquifer material)}}{\text{kg (solid)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in the ground-water zone. K_{d_q} is a site and soil-zone specific parameter depending on the fraction organic carbon in the ground-water zone or:

$$K_{d\_q} = K_{oc} \times f_{oc\_q}$$

K_{d_d}: Distribution Coefficient in Sediment Particles

The units used for K_{d_d} are $\dfrac{\text{mg/kg (dry surface-water sediment)}}{\text{mg/kg (water)}}$ and K_{d_d} is therefore unitless.

Estimation Method

This is a site specific parameter and depends on the fraction organic carbon in the surface-water sediment and the value of K_{oc}. K_{d_d} is the product of the soil organic carbon partition coefficient (K_{oc}) and the fraction of organic carbon in surface-water sediment (f_{oc_d}) [Karickhoff, 1981].

$$K_{d\_d} = K_{oc} \times f_{oc\_d}$$

$$f_{oc\_d} = \frac{\text{kg organic carbon (dry surface-water sediment)}}{\text{kg (soil)}}$$

Based on the estimation reported above, we obtain the following equation for the distribution coefficient in surface-water sediment particles. K_{d_d} is a site and soil-zone specific parameter depending on the fraction organic carbon in surface-water sediment or:

$$K_{d\_d} = K_{oc} \times f_{oc\_d}$$

K_{ps}: Partition Coefficient for Plant-Tissue (Above Ground Fresh Mass) Relative to Soil Concentration (Fresh Soil)

The units used for K_{ps} are $\dfrac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/kg (soil fresh mass [sFM])}}$ (ppm [pFM]/ppm [sFM]).

Experimental Values

0.24 to 0.49	reported at 20 to 30 °C and corresponding to a soil/foilage K_{ps} of 0.24 to 0.49 ppm (pFM)/ppm (sFM) by Wang and Jones (1994) using carrots (*Daucus Carota*), contaminated sewage sludge amended soil corresponding to 40.6 to 480 μg/kg p-DCB for 100 days and assuming plants are 20% dry mass and soil is 90% dry matter by weight

From the 2 measured values above, we obtain the following statistics for the partition coefficient in plant leaves relative to contaminant concentration in soil for *p*-DCB:

Arithmetic mean (coefficient of variation):
K_{ps} = 0.37 (0.48) ppm (pFM)/ppm (sFM)

Range: 0.24 to 0.49

Estimation Method

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:

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

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). When adjusted to a fresh-mass basis (assuming that the plant dry-mass fraction equals 0.2), this estimation equation gives the plant-soil partition coefficient, K_{ps}, expressing the ratio of contaminant concentration in mg/kg in above-ground plant fresh mass relative to contaminant concentration in mg/kg (dry soil) in the root-zone as:

$$K_{ps} = 7.7\, K_{ow}^{-0.58}\ (CV = 4.0)\ \text{ppm (pFM)/ppm (sDM)}$$

Expressing the ratio of contaminant concentration in mg/kg in above-ground plant fresh mass relative to contaminant concentration in mg/kg (fresh soil), and assuming fresh soil 10% by mass water in the root-zone soil, the K_{ps} estimation is:

$$K_{ps}\ (est) = 7.0\, K_{ow}^{-0.58}$$
$$K_{ow} = 3100$$

$$K_{ps}\ (est) = 0.067\ \text{ppm (pFM)/ppm (sFM)}$$

The estimation error reported above corresponds to a CV of 4.

K_{pa}: Biotransfer Factors For Plant Leaves Relative to Contaminant Air Concentration

The units used for K_{pa} are $\dfrac{\text{mg/kg (plant fresh mass [pFM])}}{\text{mg/cubic meter of air (m}^3\ \text{[air])}}$ $(m^3\ [a]/kg\ [pFM])$

No reported measurements of K_{pa} for *p*-DCB are available in the current literature. An estimation method for this parameter is thus applied.

Estimation Method

Based on the model of Riederer (1990) for foliar uptake of gas-phase contaminants (mg/m^3) relative to contaminant concentration in plant leaves (mg/kg fresh mass), we estimate a steady-state plant-air coefficient as:

$$K_{pa}\ (m^3\ [a]/kg\ [pFM]) = [0.5 + ((0.4 + 0.01 \times K_{ow})(RT/H))] \times 10^{-3}\ kg/m^3$$

$$R = 8.313\ \text{Pa-m}^3/\text{mol-K}$$
$$T = 298\ K$$
$$H = 260\ \text{Pa-m}^3/\text{mol}$$
$$K_{ow} = 3100$$

$$K_{pa}\ (est) = 0.29\ m^3\ [a]/kg\ [pFM]$$

McKone (1993) has estimated that the CV associated with this partition estimation model is on the order of 14.

From the estimation method identified above, we obtain the following statistics for the partition coefficient in plant leaves relative to contaminant concentration in air for p-DCB:

Arithmetic mean (coefficient of variation):
$$K_{pa} = 0.29 \ (14) \ m^3 \ [a]/kg \ [pFM]$$

BIOTRANSFER FACTORS FOR FOOD PRODUCTS

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.

B_k: Steady-State Biotransfer Factors for Whole Milk Relative to Contaminant Intake by Cattle

The units used for B_k are days/kg (milk) (d/kg [milk]).

No reported measurements of B_k are available in the current literature. Estimation methods are therefore considered.

Estimation Method 1

Based on a review of biotransfer factors for 28 organic chemicals in milk Travis and Arms (1988) developed the following geometric-mean regressions for B_{k1} based on the octanol-water partition coefficient, K_{ow},

$$\log B_{k1} = \log K_{ow} - 8.1 \pm 0.84 \ (n = 28, \ r^2 = 0.55)$$

Using the data provided by Travis and Arms (1988), we calculated the error term, ±0.84, from the mean square error of the estimator for this regression. This estimation error corresponds to a CV of 6. From the above expression and log K_{ow} of 3.49, we obtain the following statistics for the B_{k1} of p-DCB:

$$B_{k1} \ (est) = 2.4 \times 10^{-5} \ days/kg \ (milk)$$
$$CV = 6$$

Estimation Method 2

The transfer of organic chemicals from animal feed to milk 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 feed with units kg (feed)/kg (fat). Kenaga (1980) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K_{fd} to K_{ow},

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

The estimation error in this expression, ± 1, was calculated by Kenaga (1980). The above estimation error corresponds to a CV of 14. From the above expression with log K_{ow} of 3.49, an assumed pasture intake by dairy cattle of 85 kg/d (McKone and Ryan, 1989), and an assumed fat content of 0.04 in milk; we obtain the following statistics for the B_{k2} of *p*-DCB:

$$B_{k2} \text{ (est)} = 9.1 \times 10^{-6} \text{ days/kg (milk)}$$
$$CV = 14$$

The estimation values reported above yield the arithmetic mean and CV reported below:

$$B_k \text{ (avg)} = 1.7 \times 10^{-5} \text{ days/kg (milk)}$$
$$CV = 11$$

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factor for milk relative to dietary contaminant intake by dairy cattle for *p*-DCB:

Arithmetic mean (coefficient of variation):
$$B_k = 1.7 \times 10^{-5} \text{ (11) days/kg (milk)}$$

B_t: Steady-State Biotransfer Factor for Meat Relative to Contaminant Intake by Cattle

The units used for B_t are days/kg (meat) (d/kg [meat]).

No reported measurements of cattle-meat biotransfer for *p*-DCB are available in the current literature. Estimation methods are therefore considered.

Estimation Method 1

Based on a review of biotransfer factors for 36 chemicals in meat, Travis and Arms (1988) developed the following geometric-mean regression for B_{t1} based on the octanol-water partition coefficient, K_{ow},

$$\log B_{t1} = \log K_{ow} - 7.6 \pm 0.95 \ (n = 36, r^2 = 0.67)$$

Using the data provided by Travis and Arms (1988), we calculated the error term, ± 0.95 from the mean square error of the estimator for this regression. This estimation errors corresponds to a CV of 11. From the above expression and a log K_{ow} equal to 3.49, we obtain the following estimation:

$$B_{t1} \ (est) = 7.7 \times 10^{-5} \ days/kg \ (meat)$$
$$CV = 11$$

Estimation Method 2

The transfer of organic chemicals from animal feed to meat 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 feed with units kg (feed)/kg (fat). Kenaga (1980) reviewed cattle-dietary feeding studies for 23 chemicals, and from these studies derived the following fat-diet equation relating K_{fd} to K_{ow}:

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

The estimation error in this expression, ± 1, was calculated by Kenaga (1980). The above estimation error corresponds to a CV of 14. From the above expression with log K_{ow} equal to 3.49, an assumed pasture intake by beef cattle of 60 kg/d (McKone and Ryan, 1989), and an assumed fat content of 0.4 in meat; we obtain the following estimation:

$$B_{t2} \ (est) = 1.3 \times 10^{-4} \ days/kg \ (meat)$$
$$CV = 14$$

The estimation values reported above yield the arithmetic mean and CV reported below:

$$B_t \ (avg) = 1.0 \times 10^{-4} \ days/kg \ (meat)$$
$$CV = 13$$

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factor for meat relative to dietary contaminant intake by cattle for p-DCB:

Arithmetic mean (coefficient of variation):
$$B_t = 1.0 \times 10^{-4} \ (13) \ \text{days/kg (meat)}$$

B_e: Steady-State Biotransfer Factors for Eggs Relative to Dietary Contaminant Intake by Chickens

The units used for B_e are days/kg (eggs) (d/kg [eggs]).

No reported measurements of egg-diet biotransfer for p-DCB are available in the current literature. An estimation method is therefore considered.

Estimation Method

Based on measurements of polychlorodibenzodioxins (PCDDs) and polychlorodibenzo-furans (PCDFs) concentrations in soil versus concentrations in egg-fat and adipose tissue of foraging chickens, Stephens et al. (1990) have shown that contaminant concentrations in animal fat correlate with soil concentrations. In addition, they found 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 feed is higher than in the cattle feed. Based on these observation and what is discussed in the above B_k and B_t sections, we (a) assume that the fat-diet partition factor in chickens is similar to that in cattle, (b) use $\log K_{fd} = \log K_{ow} - 4.9$ 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 feed to eggs with units d/kg (eggs):

$$\log B_e = \log K_{ow} - 5.1$$
$$\log K_{ow} = 3.49$$

$$B_e = 0.024 \ \text{d/kg (eggs)}$$

We estimate the CV in this expression is 14.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated steady-state biotransfer factors for eggs relative to dietary contaminant intake by chickens for p-DCB:

Arithmetic mean (coefficient of variation):
$$B_e = 0.024 \ (14) \ \text{days/kg (eggs)}$$

B_{bmk}: Biotransfer Factor for Human Breast Milk Relative to Dietary Contaminant Intake by the Mother

The units used for B_{bmk} are days/kg (mothers milk) (d/kg [mothers milk]).

No experimental results quantifying B_{bmk} are available in the current literature. An estimation method by Smith (1987) is therefore considered:

Estimation Method

$$B_{bmk} = 2 \times 10^{-7} \, K_{ow}$$

$$K_{ow} = 3100$$

$$B_{bmk} = 6.2 \times 10^{-4} \text{ days/kg (mothers milk)}$$

The CV of the above estimation method is approximately 10.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated biotransfer factor for human breast milk concentration relative to dietary contaminant intake by the mother for *p*-DCB:

Arithmetic mean (coefficient of variation):
$$B_{bmk} = 6.2 \times 10^{-4} \text{ (10) days/kg (mothers milk)}$$

BCF: Bioconcentration Factors for Fish Relative to Water Concentration

The units used for BCF (fish/water) are $\dfrac{\text{mg/kg (fish)}}{\text{mg/liter (water)}}$, and BCF is therefore unitless.

Experimental Values:

50	reported as a fish BCF of 50 by Freitag et al. (1985) using Golden Ide (*Idus idus melanotus*) for 3 days
60	reported at 16 °C as a fish/water BCF of 60 by Veith et al. (1980) using bluegill sunfish (*Lepomis machrochirus*) and a concentration of 10.1 ug/l
72	reported at 11 °C as a fish lipid BCF of 3,147 by Galassi (1982) using 56 day old rainbow trout (*Salmo gaidneri*) alevins (2.3% lipid) in two 48 hr. tests at 15.5 μg/L
97	reported at 25 °C as a fish BCF (fat wt.) of 1800 by Konemann and van Leeuwen (1980) using guppies [*Poecilia reticulata* (5.4% fat)] at 160 ppb for 19 days in a closed flow-through system

107   reported as a fish lipid log BCF of 3.51 by Periera et al. (1988) using field collected blue catfish [Ichtalurus furcatus (3.3% lipid)] from the Calcasieu River estuary, Louisiana

110   reported at 25 °C as a fish BCF of 110 by Carlson and Kosian (1987) using fathead minnow (*Pimephles promelas*) at 570 and 1000 ppb for 32 days in filtered Lake Superior water (pH = 7.4)

215   reported as a trout muscle/water BCF of 215 by Neely et al. (1974) using *Salmo gairdneri* at 54 °F [Also cited in Mackay et al. (1993)]

226   reported as a fish BCF of 226 by Calamari et al. (1982) using data from *Salmo gaidneri* alevins aged 30 to 60 days after lifetime treatment at 3 µg/L

283   reported as a fish lipid log BCF of 4.09 by Periera et al. (1988) using field collected spotted sea trout [Ichtalurus furcatus (2.3% lipid)] from the Calcasieu River estuary, Louisiana

296   reported at 25 °C as an average fish BCF of 296 by Smith et al. (1990) using American Flagfish (*Jordanella floridae*), aged 4-6 months with 8.5% lipid content, for 28 days at 5 µg/L p-DCB in flow-through test chambers

370 to 720   reported at 15 °C as a fish BCF of 370 and 720 by Oliver and Niimi (1983) using rainbow trout (*Salmo gairdneri*) and Lake Ontario water at 28 and 670 ppb p-DCB respectively

510 to 890   reported at 15 °C as a fish BCF of 510 and 890 by Oliver and Niimi (1985) using 200g rainbow trout (*Salmo gairdneri*) in flow-through tanks for 96 days and at 81 and 73 ppb p-DCB respectively

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From the 14 measured values reported above, we obtain the following statistics for BCF in fish relative to contaminant concentration in water for *p*-DCB:

Arithmetic mean (coefficient of variation):
BCF (fish/water) = 290 (0.90)

Range: 50 to 890

Estimation Method

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:

$$BCF = 0.048\ K_{ow}$$
$$K_{ow} = 3100$$

BCF (est) = 150

CV = 0.60

The reported GSD is 1.8 which corresponds to an estimation error of 0.6 but does not include the error associated with the K_{ow}.

K_{p_w}: Human Skin Permeability Coefficient Relative to Contaminant Concentration in Water

The units used for K_{p_w} are centimeters/hour (cm/hr).

No reported measurements of K_{p_w} for p-DCB are available in the current literature. An estimation method for this parameter is thus applied.

Estimation Method

Because dermal transfer is considered a nonsteady-state event, diffusion models require input parameters which are difficult to measure, such as the stratum corneum diffusion coefficient (D_{sc}) [Flynn and Amidon, 1991]. Estimation of aqueous biotransfer of p-DCB is calculated with the following equation based on the estimation method of McKone and Howd (1992).

$$K_{p\_w} = MW^{-0.6} \left[0.33 + \frac{0.0025}{2.4 \times 10^{-6} + 3 \times 10^{-5} \, K_{ow}^{0.8}} \right]^{-1}$$

$K_{ow} = 3100$

MW = 147 g/mol

$K_{p\_w} = 0.11$ cm/hr

who report a coefficient of variation equal to 2.4

Based on the estimation equation and the estimation error reported above, we obtain the following value for the estimated human skin permeability coefficient relative to contaminant water concentration for p-DCB:

Arithmetic mean (coefficient of variation):
$K_{p\_w} = 0.11$ (2.4) cm/hr

K_m: Partition Coefficient for Human Skin Relative to Contaminant Concentration in Water or Soil

The units used for K_m are $\dfrac{\text{mg/kg (skin)}}{\text{mg/liter (water)}}$ (ppm [skin]/ppm [water]).

No experimental values for K_m are currently available in the literature, therefore an estimation method is considered.

Estimation Method

Experimental values quantifying dermal transfer of *p*-DCB in water, or for water in a soil matrix, may depend on pH, particle size and organic carbon content (Flynn and Amidon, 1991). An estimation method based on McKone and Howd (1992) is therefore used here.

$$K_m = 0.64 + (0.25\ K_{ow}^{0.8})$$

$$K_{ow} = 3100$$

$$K_m = 150 \text{ ppm (skin)/ppm (water)}$$

The reported geometric standard deviation of 1.3 in this estimation method corresponds to a CV of 0.27.

Based on the estimation equation and the estimation error reported above, we obtain the following value for the partition coefficient into human skin relative to *p*-DCB water or soil concentration:

Arithmetic mean (coefficient of variation):
K_m= 150 (0.27) ppm (skin)/ppm (water)

T_{half_a}: Reaction Half-Life in Air

The units used for T_{half_a} are days.

3	reported as a reaction rate constant in air of 9.63×10^{-3} hr^{-1} by Ware and West (1977) [also cited in Mackay et al. (1993)]
25	reported at 22 °C as a reaction rate constant of 3.2×10^{-13} cm^3/molecule-sec by Wahner and Zetzsch (1983) using 133 millibar [AR] and assuming a hydroxyl radical concentration of 1×10^6 molecules/cm^3

From the 2 experimental values reported above, and the assumption that the actual range of half-lives may be a factor of 5 higher or lower than this range, we obtain the following statistics on the reaction half-life for p-DCB in air:

> Arithmetic mean (coefficient of variation):
> T_{half_a} = 38 (1.5) days

Range: 0.6 to 125 days

T_{half_g}: Reaction Half-Life in Ground-Surface Soil

The units used for T_{half_g} are days.

Reported Values

185 to 774	reported at 20 to 30 °C and corresponding to a soil degradation half-life of 185 to 774 days by Wang and Jones (1994) using contaminated sewage sludge amended soil corresponding to 40.6 to 480 µg/kg p-DCB for 100 days and assuming first-order degradation
265	reported as a degradation in soil of 47% in 241 days by Demirjian et al. (1987) using a sludge amended Ribicon soil tilled to a 6" depth, 430 µg benzene/kg soil and assuming first-order kinetics
640	reported as a degradation half-life of 6.3% in 10 weeks by Haider et al. (1981) using a para-brownish soil from Flachstockheim, 2 mg/100 g soil and assuming first-order degradation
745	reported as 6.3% degradation in 10 weeks by Bailey et al. (1974) using para-brown soil (f_{oc} = 1.26%, pH = 1.7) at 20 ppm and assuming first-order degradation

From the 5 values above, we obtain the following statistics for the reaction half-life for p-DCB in surface soil:

> Arithmetic mean (coefficient of variation):
> T_{half_g} = 520 (0.53) days

Range: 185 to 774 days

T_{half_s}: Reaction Half-Life in Root-Zone Soil

The units used for T_{half_s} are days.

Reported Values

185 to 774	reported at 20 to 30 °C and corresponding to a soil degradation half-life of 185 to 774 days by Wang and Jones (1994) using contaminated sewage sludge amended soil corresponding to 40.6 to 480 µg/kg p-DCB for 100 days and assuming first-order degradation
265	reported as a degradation in soil of 47% in 241 days by Demirjian et al. (1987) using a sludge amended Ribicon soil tilled to a 6" depth, 430 µg benzene/kg soil and assuming first-order kinetics
640	reported as a degradation half-life of 6.3% in 10 weeks by Haider et al. (1981) using a para-brownish soil from Flachstockheim, 2 mg/100 g soil and assuming first-order degradation
745	reported as 6.3% degradation in 10 weeks by Bailey et al. (1974) using para-brown soil (f_{oc} = 1.26%, pH = 1.7) at 20 ppm and assuming first-order degradation

From the 5 values above, we obtain the following statistics for the reaction half-life for *p*-DCB in root-zone soil:

Arithmetic mean (coefficient of variation):
T_{half_s} = 520 (0.53) days

Range: 185 to 774 days

T_{half_v}: Reaction Half-Life in Vadose-Zone Soil

The units used for T_{half_v} are days.

Reported Values

185 to 774	reported at 20 to 30 °C and corresponding to a soil degradation half-life of 185 to 774 days by Wang and Jones (1994) using contaminated sewage sludge amended soil corresponding to 40.6 to 480 µg/kg p-DCB for 100 days and assuming first-order degradation
265	reported as a degradation in soil of 47% in 241 days by Demirjian et al. (1987) using a sludge amended Ribicon soil tilled to a 6" depth, 430 µg benzene/kg soil and assuming first-order kinetics
640	reported as a degradation half-life of 6.3% in 10 weeks by Haider et al. (1981) using a para-brownish soil from Flachstockheim, 2 mg/100 g soil and assuming first-order degradation

745   reported as 6.3% degradation in 10 weeks by Bailey et al. (1974) using para-brown soil (f_{oc} = 1.26%, pH = 1.7) at 20 ppm and assuming first-order degradation

> From the 5 values above, we obtain the following statistics for the reaction half-life for p-DCB in vadose-zone soil:
>
> Arithmetic mean (coefficient of variation):
> T_{half_v} = 520 (0.53) days

Range: 185 to 774 days

T_{half_q}: Reaction Half-Life in Groundwater

The units used for T_{half_q} are days.

Reported Values

10   reported at 20 °C as as a degradation half-life of approximately 10 days by Kuhn et al. (1985) using an aquifer material incubated with an aerobic xylene adapted culture at 0.2 μM in the dark and assuming first-order degradation

56 to
365   reported as an estimated unacclimated aqueous aerobic biodegradation half-life of 8 to 12 months by Howard et al. (1990) using aerobic data from Canton et al. (1985) and Haider et al. (1981)

> From the 3 values above, and the assumption that the actual range of half-lives may be a factor of 5 higher and lower than this range, we obtain the following statistics for the reaction half-life for p-DCB in ground-water zone material:
>
> Arithmetic mean (coefficient of variation):
> T_{half_q} = 450 (1.7) days

Range: 2 to 1820 days

T_{half_w}: Reaction Half-Life in Surface Water

The units used for T_{half_w} are days.

Reported Values

0.26 to
1.1   reported at 25 °C as an aquatic photolysis degradation rate constant of 0.7 to 3.1×10^{-5} sec-1 by Mansour et al. (1989) using distilled and filtered river water, 7.8×10^{-4} mol/L and assuming a first-order degradation

7	reported at 25 °C as a half-life in water of 7 days by Tabak et al. (1981) using domestic wastewater conditions in a static-culture flask-screening procedure for 28 days in the dark
24 to 26	reported as a first order degradation half-life of 24 to 26 days reported by Zoetemann et al. (1980) and based on the concentration reduction between sample points on the Rhine River and a lake in the Rhine basin [also cited in Mackay et al. (1993)]

From the 4 values above, we obtain the following statistics for the half-life for p-DCB in surface water at 25 °C:

Arithmetic mean (coefficient of variation):
T_{half_w} = 12 (1.1) days

Range: 0.26 to 26 days

T_{half_d}: Reaction Half-Life in Surface Water Sediment

The units used for T_{half_d} are days.

Reported Values

7	reported at 25 °C as a half-life in water of 7 days by Tabak et al. (1981) using domestic wastewater conditions in a static-culture flask-screening procedure for 28 days in the dark
24 to 26	reported as a first order degradation half-life of 24 to 26 days reported by Zoetemann et al. (1980) and based on the concentration reduction between sample points on the Rhine River and a lake in the Rhine basin [also cited in Mackay et al. (1993)]
112 to 720	reported as an estimated anaerobic biodegradation half-life of 2699 to 17280 hours by Howard et al. (1990) using scientific judgement and an estimated aqueous unacclimated biodegradation half-life from data measured by Canton et al. (1985) and Haider et al. (1981)

From the 5 values above, we obtain the following statistics for the reaction half-life for p-DCB in surface water sediment:

Arithmetic mean (coefficient of variation):
T_{half_d} = 180 (1.7) days

Range: 7 to 720 days

References

Agency for Toxic Substances and Disease Registry, 1989. *Toxicological Profile for 1,4-Dichlorobenzene*, PB89-160352

Andrews, L.J., and R.M. Keefer, 1950. Cation Complexes of Compounds Containing Carbon-Carbon Double Bonds. VII. Further Studies on the Argentation of Substituted Benzenes, *J. Am. Chem. Soc.* 72:5034-5037

Aquan-Yuen, M., D. Mackay and W.Y. Shiu, 1979. Solubility of Hexane, Phenanthrene, Chlorobenzene, and *p*-Dichlorobenzene in Aqueous Electrolyte Solutions, *J. Chem. Eng. Data* 24(1):30-34

Ashworth, R. A., Howe, G. B., Mullins, M. E., and Rogers, T. N., 1988. Air-Water Partitioning Coefficients of Organics in Dilute Aqueous Solutions, *J. Haz. Mater.* 18:25-36

Atchison, J. and J.A.C. Brown, 1957. *The Lognormal Distribution,* Cambridge University; New York, NY. pp 125

Atkinson, R. and W. P. Carter, 1984. Kinetics and Mechanisms of the Gas-Phase Reactions of Ozone with Organic Compounds under Atmospheric Conditions, *Chem Rev.* 84:437-470

Bailey, R.E., 1983. Comment on "Chlorobenzenes in Sediments, Water, and Selected Fish From Lakes Superior, Huron, Erie, and Ontario", *Environ. Sci. Technol.* 17:504

Banerjee, S., 1984. Solubility of Organic Mixtures in Water, *Environ. Sci. Technol.* 18(8):587-591

Banerjee, S., S.H. Yalkowsky, and S.C. Valvani 1980. Water Solubility and Octanol/Water Partition Coefficient of Organics. Limitations of Solubility-Partition Coefficient Correlation, *Environ. Sci. Technol.* 14(10):1227-1229

Boublík, T., V. Fried, and E. Hála, 1984. *The Vapour Pressures of Pure Substances: Selected Values of the Temperature Dependence of the Vapour Pressures of Some Pure Substances in the Normal and Low Pressure Region,* 2nd Revised ed., Physical Sciences Data 17. Elsevier Science; Amsterdam, The Netherlands

Calamari, D., S. Galassi and F. Setti, 1982. Evaluating The Hazard of Organic Substances on Aquatic Life: The Paradichlorobenzene Example, *Ecotoxicol. Environ. Saf.* 6: 369-378

Canton, J.H., W. Slooff, H.J. Kool, J. Struys, Th.J.M. Pouw, R.C.C. Wegman and G.J. Piet, 1985. Toxicity, Biodegradability, and Accumulation of a Number of Cl/N-Containing Compounds for Classification and Establishing Water Quality Criteria, *Regul. Toxicol. Pharmacol.* 5:123-131

Carlson, A.R., and P.A. Kosian, 1987. Toxicity of Chlorinated Benzenes to Fathead Minnows (*Pimephales promelas*), *Arch. Environ. Contam. Toxicol.* 16:129-135

Chiou, C.T., and T.D. Shoup, 1985. Soil Sorption of Organic Vapors and Effects of Humidity on Sorptive Mechanism and Capacity, *Environ. Sci. Technol.* 19(12):1196-1200

Chiou, C.T., P.E. Porter and D.W. Schmedding, 1983. Partition Equilibria of Nonionic Organic Compounds between Soil Organic Matter and Water, *Environ. Sci. Technol.* 17:227-231

Clayton, G. D. and Clayton, F. E. Ed., 1981. *Patty's Industrial Hygiene & Toxicology.* Third ed., John Wiley & Sons; New York, NY. Vol. 2B:3491-3497

Cornelis, A. M., van Gestel, Wei-chun Ma and C. Els Smit, 1991. Development of QSAR's in Terrestrial Ecotoxicology: Earthworm Toxicity and Soil Sorption of Chlorophenols, Chlorobenzenes and Dichloroaniline; *The Science of the Total Environment,* **109/110:589-604**

Darkis, F.R., H.E. Vermillion and P.M. Gross, 1940. p-Dichlorobenzene as a Vapor Fumigant: Physical and Chemical Studies, *Indus. Eng. Chem.* **32(7):946-949**

Daubert, T. E. and R. P. Danner, 1985. *Data Compilation of Pure Compounds*, Vol. I, July 1985. Design Institute for Physical Property Data. American Institute of Chemical Engineers, 345 East 47th Street, New York, NY

Daubert, T. E. and R. P. Danner, 1989. *Data Compilation of Pure Compounds*, Vol. II, Design Institute for Physical Property Data. American Institute of Chemical Engineers, 345 East 47th Street; New York, NY

De Bruijn, J., F. Busser, W. Seinen and J. Hermens, 1989. Determination of Octanol/Water Partition Coefficients for Hydrophobic Organic Chemicals with the Slow-Stirring Method, *Environ. Toxicol. Chem.* **8:499-512**

Dean, J.D., Ed. 1985. *Lange's Handbook of Chemistry,* McGraw-Hill; New York, NY, **13th ed**

Dreisbach, R., 1959. *Advances in Chemistry Series (22): Physical Properties of Chemical Compounds--II,* American Chemical Society; Washington, DC407

Flynn and Amidon, 1991. *Dermal Exposure Assessment: Principles and Applications*, Interim Report. USEPA Jan, 1992. Office of Research and Development; Washington, DC. EPA/600/8-91/011B

Freed, V. H., Chiou, C. T., Schmedding, D., and R. Kohnert, 1979. Some Physical Factors in Toxicological Assessment Tests, *Environ. Health Perspect.*, **30:75-80**

Freitag, D., L. Ballhorn, H. Geyer and F. Korte, 1985. Environmental Hazard Profile of Organic Chemicals, *Chemosphere* **14(10):1589-1616**

Friesel, P., G. Milde and B. Steiner, 1984. Interactions of Halogenated Hydrocarbons with Soils, *Fresenius Z. Anal. Chem.* **319:160-164**

Fuller, E.N., P.D. Schettler, and J.C. Giddings, 1966. A New Method for Prediction of Binary Gas-Phase Diffusion Coefficients, *Ind. Eng. Chem.* **58:19-27**

Galassi, S., D. Calamari and F. Setti, 1982. Uptake and Release of p-Dichlorobenzene in Early Life Stages of <u>Salmo gairdneri</u>, *Ecotoxicol. Environ. Saf.* **6:439-447**

Gossett, J.M. 1987. Measurement of Henry's Law Constants for C_1 and C_2 Chlorinated Hydrocarbons, *Environ. Sci. Technol.* **21:202–208**

Gross, P.M., and J.H. Saylor, 1931. The Solubilities of Certain Slightly Soluble Organic Compounds in Water, *J. Am. Chem. Soc.* **53:1744-1751**

Haider, K., G. Jagnow, R. Kohnen and S.U. Lim, 1981. Degradation of Chlorinated Benzenes, Phenols and Cyclohexane Derivatives by Benzene and Phenol-Utilizing Soil Bacteria Under Aerobic Conditions: Decomposition of Toxic and Nontoxic Organic Compounds in Soils, Ann Arbor Science; Ann Arbor, MI. pp 207-223

Hamburg, M. 1970. *Statistical Analysis for Decision Making*, Harcourt Brace Jovanovich; San Diego, CA

Hammers, W.E., G.J. Meurs and C.L. De Ligny, 1982. Correlations Between Liquid Chromatographic Capacity Ratio Data on Lichrosorb RP-18 and Partition Coefficients in the Octanol-Water System, *J. Chromatog.* **247:1-13**

Hansch, C., and A. Leo, 1985. The Log P and Related Parameters Database, created and updated by the Medicinal Chemistry Project at Pomona College under the direction of Corwin Hansch and Albert Leo — 1985 Printout, *Medchem Project Issue Nº. 26,* Pomona College; Claremont, CA

Hansch, C., and A. Leo, 1987. The Log P and Related Parameters Database, created and updated by the Medicinal Chemistry Project at Pomona College, Claremont, CA, under the direction of Corwin Hansch and Albert Leo — 1987 Printout.

Horvath, A. L., 1982. *Halogenated Hydrocarbons, Solubility–Miscibility with Water* Marcel Dekker; New York, NY

Howard, P. H., R. S. Boethling, W. F. Jarvis, W. M. Meylan, and E. M. Michalenko Eds., 1991. *Handbook of Environmental Degradation Rates* Lewis; Chelsea, MI

Howard, P.H., G.W. Sage, W.F. Jarvis, and D.A. Gray, Eds. 1990. *Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Volume II. Solvents* Lewis; Chelsea, MI

Kenaga, E. E., 1980. Correlation of Bioconcentration Factors of Chemicals in Aquatic and Terrestrial Organisms with their Physical and Chemical Properties, *Environ. Sci. Technol.* **14(5):553-556**

Kirk-Othmer Encyclopedia of Chemical Technology. 1985. Wiley-Interscience, John Wiley & Sons; New York, NY. 3rd ed., Vol. 5

Kirk–Othmer Encyclopedia of Chemical Technology, 1964. *Chlorocarbons and Chlorohydrocarbons*, Wiley Interscience; New York, NY. ,2nd ed., Vol. 5, pp 100-363

Konemann, H., and K. van Leeuwen, 1980. Toxicokinetics in Fish: Accumumulation and Elimination of Six Chlorobenzenes by Guppies, *Chemosphere* **9:3-19**

Konemann, H., R. Zelle, F. Busser and W.E. Hammers, 1979. Determination of Log P Oct Values of Chloro-Substituted Benzenes, Toluenes and Anilines by High-Performance Liquid Chromatography on ODS-Silica. *J. Chrom.* **178:559-565**

Kuhn, E.P., P.J. Colberg, J.L. Schnoor, O. Wanner, A.J.B. Zehnder and R.P. Schwarzenbach, 1985. Microbial Transformations of Substituted Benzenes During Infiltration of River Water to Groundwater: Laboratory Column Studies, *Environ. Sci. Technol.* **19:961-968**

Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt, 1982. *Handbook of Chemical Property Estimation Methods:* Environmental Behavior of Organic Compounds, American Chemical Society; Washington, DC

Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt, 1990. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds,* American Chemical Society; Washington, DC

Mackay, D. 1982. Correlation of Bioconcentration Factors, *Environ. Sci. Technol.* **16:274–278**

Mackay, D., W. Y. Shiu, and K. L. Ma, 1992. *Illustrated Handbook of Physical Chemical Properties and Environmental Fate for Organic Chemicals. Vol. II. Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans,* Lewis; Boca Raton, FL

Mackay, D., W.-Y. Shiu, and K.-C. Ma, 1993. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume III. Volatile Organic Chemicals,* Lewis; Boca Raton, FL

Mansour, M., E. Feicht and P. Meallier, 1989. Improvement of the Photostability of Selected Substances in Aqueous Medium, *Toxicol. Environ. Chem.* 20/21:139-147

McDonald, R.A., S.A. Shrader and D.R. Stull, 1959. Vapor Pressures and Freezing Points of 30 Organics, *J. Chem. Eng. Data* 4(4):311-313

McGovern, E. W. 1943. Chlorohydrocarbon Solvents, *Ind. Eng. Chem.* 35(12):1230-1239

McKone, T. E., and P. B. Ryan, 1989. Human Exposures to Chemicals Through Food Chains: An Uncertainty Analysis, *Environ. Sci. Technol.* 23:1154-1163

McKone, T. E., and R. A. Howd, 1992. Estimation Dermal Uptake of Nonionic Organic Chemicals from Water and Soil: I. Unified Fugacity-Based Models for Risk Assessments, *Risk Analysis* 12(4):543-557

McKone, T.E., 1993. The Precision of QSAR Methods for Estimating Intermedia Transfer Factors in Exposure Assessments, *SAR and QSAR in Environmental Research,* 1:41-51

Miller, M.M., S. Ghodbane, S.P. Wasik, Y.B. Tewari and D.E. Martire, 1984. Aqueous Solubilities, Octanol/Water Partition Coefficients, and Entropies of Melting of Chlorinated Benzenes and Biphenyls, *J. Chem. Eng. Data* 29:184-190

Miller, M.M., S.P. Wasik, G.L. Huang, W.Y. Shiu and D. Mackay, 1985. Relationships Between Octanol-Water Partition Coefficient and Aqueous Solubility, *Environ. Sci. Technol.* 19:6 522-529

Neely, W.B., D.R. Branson, and G.E. Blau, 1974. Partition Coefficient to Measure Bioconcentration Potential of Organic Chemicals in Fish, *Environ. Sci. Technol.* 8:1113–1115

Oliver, B. G., and A. J. Niimi, 1985. Bioconcentration Factors of Some Halogenated Organics for Rainbow Trout, *Environ. Sci. Technol.* 19:842-849

Oliver, B.G., 1985. Desorption of Chlorinated Hydrocarbons from Spiked and Anthropogenically Contaminated Sediments, *Chemosphere* 14(8):1087-1106

Oliver, B.G., and A.J. Niimi, 1983. Bioconcentration of Chlorobenzenes from Water by Rainbow Trout: Correlations with Partition Coefficients and Environmental Residues, *Environ. Sci. Technol.* 17:287-291

Oliver, B.G., and M.N. Charlton, 1984. Chlorinated Organic Contaminants on Settling Particulates in The Niagara River Vicinity of Lake Ontario, *Environ. Sci. Technol.* 18:903-908

Periera, W. E., Rostad, C. E., Chiou, C. T., Brinton, T. I., Barber, L. B. II, Demcheck, K., and C. R. Demas, 1988. Contamination of Estuarine Water, Biota, and Sediment by Halogenated Organic Compouds: A Field Study. *Environ. Sci. Technol.* 22:772-778.

Reid, R. C., J. M. Prausnitz, and B. E. Poling, 1987. *The Properties of Gases and Liquids* McGraw Hill; New York, NY. 4th ed

Reiderer, M. 1990. Estimating Partitioning and Transport of Organic Chemicals in the Foliage/Atmosphere System: Discussion of a Fugacity-Based Model, *Environ. Sci. Technol.* **24:829–837.**

Reiderer, M., 1990. Estimating Partitioning and Transport of Organic Chemicals in the Foliage/Atmosphere System: Discussion of a Fugacity-Based Model, *Environ. Sci. Technol.* **24:829–837**

Riddick, J. A., Bunger, W. B., and T. K. Sakano, 1986. *Organic Solvents: Physical Properties and Mehods of Purification,* John Wiley & Sons; New York, NY. 4th ed., Vol. II, No. 319

Sax, N. I. and R. J. Lewis Sr., 1989. *Dangerous Properties of Industrial Materials*. 7th Ed., Van Nostrand Reinhold; New York, NY

Smith, A. H. 1987. Infant Exposure Assessment for Breast Milk Dioxins and Furans Derived from Waste Incineration Emissions, *Risk Analysis* 7:347-353.

Smith, A.D., A. Bharath, C. Mallard, D. Orr, L.S. McCarty and G.W. Ozburn, 1990. Bioconcentration Kinetics of Some Chlorinated Benzenes and Chlorinated Phenols in American Flagfish, *Jordanella floridae* (Goode and Bean), Chemosphere 20(3/4):379-386

Southworth, G.R., and J.L. Keller, 1986. Hydrophobic Sorption of Polar Organics by Low Organic Carbon Soils, *Water Air Soil Poll.* **28:239-248**

Stephens, R. D., Harnly, M., Haywood, G. G., Chang, R. R., Flattery, J., Petreas, M. X., Goldman, L., 1990. Bioaccumulation of Dioxins in Food Animals II: Controlled Exposure Studies, *Chemosphere* 20:1091-1096

Stull, D. R. 1947. Vapor Pressure of Pure Substances: Organic Compounds, *Ind. Eng. Chem.* **39:517–540**

Tabak, H. H., Quave, S. A., Mashni, C. I., and Barth, E. F., 1981. Biodegradability Studies with Organic Priority Pollutant Compounds, *J. Water Pollut. Control Fed.* 53:153-1518

Topp, E., Scheunert, I., Attar, A. and F. Korte, 1986. Factors Affecting the Uptake of ^{14}C-Labeled Organic Chemicals by Plants from Soil, *EcoToxicol. Environ. Saf.* **11:219–228**

Travis C. C., Hattemer-Frey, H. A., and A. D. Arms, 1988. Relationship Between Dietary Intake of Organic Chemicals and their Concentrations in Human Adipose Tissue and Breast Milk, *Chemosphere* 17: 277-284

Travis, C. C., and A. D. Arms, 1988. Bioconcentration of Organics in Beef, Milk, and Vegetation, *Environ. Sci. Technol.* **22:271–274.**

Uchrin, C.G., and J. Katz, 1986. Sorption Kinetics of Completing Organic Substances on New Jersey Coastal Plain Aquifer Solids: Hazardous and Industrial Solid Waste Testing and Disposal (ASTM Special Technical Publication 933)American Society for Testing and Materials; Philadelphia, PA Vol. 6, pp 140-150

Veith, G.D., K.J. Macek, S.R. Petrocelli, and J. Caroll, 1980. "An Evaluation of Using Partition Coefficients and Water Solubility to Estimate Bioconcentration Factors for Organic Chemicals in Fish", in: *Aquatic Toxicology, ASTM STP 707,* J. G. Eaton, P. R. Parrish, and A. C. Hendricks, Eds. American Society for Testing and Materials; Philadelphia, PA. pp 117–119

Verscheuren, K., 1977. *Handbook of Environmental Data on Organic Chemicals* , Van Nostrand/Reinhold; New York, NY

Verschueren, K., 1983. *Handbook of Environmental Data on Organic Chemicals,* Second ed.,Van Nostrand/Reinhold; New York, NY

Vesala, A., 1974. Thermodynamics of Transfer of Nonelectrolytes from Light to Heavy Water I: Linear Free Energy Correlations of Free Energy of Transfer with Solubility and Heat of Melting of a Nonelectrolyte, *Acta Chem. Scand.* 28:839-845

Wahner, A., and C. Zetzsch, 1983. Rate Constants For The Addition of OH to Aromatics (Benzene, p-Chloroaniline, and o-,m-, and p-Dichlorobenzene) And the Unimolecular Decay of The Adduct, Kinetics into a Quasi-Equilibrium I. *J. Phys. Chem.* 87: 4945-4951

Walsh, P.N., and N.O. Smith, 1961. Sublimation Pressure of Alpha-p-dichloro, Beta-p-dichloro, p-Dibromo, and p-Bromochlorobenzene, *J. Chem. Eng. Data* 6(1):3-35

Wang, M. J., and K. C. Jones, 1994. Uptake of Chlorobenzenes by Carrots from Spiked and Sewage Sludge-Amended Soil, *Environ. Sci. Technol.* 28:1260-1267

Ware, W. and W. West, 1977. Investigation of Selected Potential Environmental Contaminants-Halogenated Benzenes, EPA 560/2-77-004

Wasik, S.P., Y.B. Tewari, M.M. Miller and D.E. Martire, 1981. :*Octanol/Water Partition Coefficients and Aqueous Solubilities of Organic Compounds.* NBSIR No. 81-2406 U.S. Dept. of Commerce, National Bureau of Standards, Washington DC pp 67

Wataral, H., M. Tanaka and N. Suzuki, 1982. Determination of Partition Coefficients of Halobenzenes in Heptane/Water and 1-Octanol/Water Systems and Comparison with the Scaled Particle Calculation. *Anal. Chem.* 54:702-705

Wauchope, R.D., and F.W. Getzen, 1972. Temperature Dependence of Solubilities in Water and Heats of Fusion of Soild Aromatic Hydrocarbons, *J. Chem. Eng. Data* 17(1):38-41

Weast, R. C., Astle, M.J. and Beyer, W.H. Eds., 1983. *CRC Handbook of Chemistry and Physics: A Ready Reference Book of Chemical and Physical Data,* 63rd ed., CRC; Boca Raton, FL

Weast, R. C., Lide, D. R., Astle, M.J. and Beyer, W.H., Eds. 1989. *CRC Handbook of Chemistry and Physics: A Ready Reference Book of Chemical and Physical Data,* 67th ed. CRC Press; Boca Raton, FL

Wilke, C.R., and P. Chang, 1955. Correlation of Diffusion Coefficients in Dilute Solutions, *AIChE J.* 1:264–270

Wilson, B. H., Smith G. B., and J. F., Rees, 1986. Biotransformations of Selected Alkylbenzenes and Halogenated Aliphatic Hydrocarbons in Methanogenic Aquifer Material: A Microcosm Study, *Environ. Sci. Technol.,* 20(10):997-1002

Windholz, M., S. Budavari, R. F. Blumetti, and E. S. Otterbein, Eds., 1983. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals, 10th Ed.* Merck; Rahway, NJ.

World Health Organization International Agency for Research on Cancer, 1982. IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans: Some Industrial Chemicals and Dyestuffs, Vol. 29, 13-20 October 1981

Yalkowsky, S.H., and S.C. Valvani, 1980. Solubility and Partitioning I: Solubility of Nonelectrolytes in Water, *J. Pharm. Sci.* **69(8):912-922**

Yurteri, C., D.F. Ryan, J.J. Callow and M.D. Gurol, 1987. The Effect of Chemical Composition of Water on Henry's Law Constant, *J. Water Pollut. Control Fed.* **59:950-956**

Zoeteman, B.C.J., Harmsen, K., Linders, J. B. H. J., Morra, C. F. H., and W. Slooff, 1980. Persistent Organic Pollutants in River Water and Groundwater of the Netherlands, *Chemosphere* **9:231–249**