# APPENDIX A

# CHEMICAL-SPECIFIC DATA

## DELISTING TECHNICAL SUPPORT DOCUMENT

**August 2000**

U.S. EPA Region 6
Multimedia Planning and Permitting Division
RCRA Delisting Team
and
U.S. EPA
Office of Solid Waste

**A-1 CHEMICAL DATA FOR WASTE CONSTITUENTS IN DRAS PROGRAM**

**A-2 NATIONAL PRIMARY DRINKING WATER STANDARDS**

**A-3 SOIL SATURATION VALUES**

**A-4 TARGET ORGANS AND CRITICAL EFFECTS FOR COMPOUNDS WITH REFERENCE DOSES**

**A-5 DEFAULT VARIABLES: ABBREVIATIONS, UNITS, AND VALUES**

# APPENDIX A-1

## CHEMICAL INFORMATION ON DRAS WASTE CONSTITUENTS

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**Attachment**

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

## APPENDIX A-1

## LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

| | | |
|---|---|---|
| *Aquatic TRV* | = | Ambient Water Quality Criteria (µg/L) |
| *B* | = | Bunge constant (unitless) |
| $BAF_{fish}$ | = | Bioaccumulation factor in fish<br>(mg Chemical/kg FW tissue)/(mg Chemical/L total water column)<br>OR (L water/kg FW tissue) |
| $BCF_{fish}$ | = | Bioconcentration factor in fish (L/kg FW OR unitless) |
| $D_a$ | = | Diffusivity of Chemical in air ($cm^2/s$) |
| $D_w$ | = | Diffusivity of Chemical in water ($cm^2/s$) |
| *H* | = | Henry's law constant |
| *Inhalation CSF* | = | Inhalation cancer slope factor $(mg/kg\text{-}day)^{-1}$ |
| $Kd_s$ | = | Soil-water partition coefficient (L water/g soil OR $cm^3$ water/g soil) |
| $Kd_{sw}$ | = | Suspended sediment-surface water partition coefficient<br>(mL water/g bottom sediment OR $cm^3$ water/g bottom sediment) |
| $K_{ow}$ | = | Octanol/water partitioning coefficient<br>(mg Chemical/L octanol)/(mg Chemical/L octanol)—unitless |
| $K_{oc}$ | = | Soil organic carbon-water partition coefficient (mL water/g soil) |
| $K_P{}^w$ | = | Skin permeability constant in water (cm/hr) |
| *MCL* | = | National Primary Drinking Water Regulation (mg/L) |
| *MW* | = | Molecular weight of Chemical (g/mole) |
| *Oral CSF* | = | Oral cancer slope factor $(mg/kg\text{-}day)^{-1}$ |
| *RfC* | = | Reference concentration ($mg/m^3$) |
| *RfD* | = | Reference dose (mg/kg/day) |
| *Sol* | = | Solubility of Chemical in water (mg Chemical/L water) |
| $\tau$ | = | Lag time (hr) |
| $t^*$ | = | Time to skin permeability steady state (hr/event) |
| $T_m$ | = | Melting point temperature (K) |
| $V_p$ | = | Vapor pressure of Chemical (atm) |

# APPENDIX A-1

The following sections provide the methodology and rationale followed for the selection or development of compound-specific parameter values recommended by U.S. EPA OSW. Compound-specific values are provided for (1) physical and chemical properties, (2) fate-and-transport parameters, and (3) health benchmarks. A summary table of all compound-specific parameter values is provided at the end of this appendix, followed by individual parameter-value tables for each compound. The individual parameter-value tables cite sources for each parameter value.

## A.1.1 COMPOUND NAME with CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The Appendix A-1 Tables of waste constituents included in the Delisting Risk Assessment Software (DRAS) program are lists the chemicals by most common compound name. The CAS number provided in parenthesis is a unique number assigned to each compound in the table.

## A.1.2 PHYSICAL AND CHEMICAL PROPERTIES

### Molecular Weight (*MW*)

Molecular weight (*MW*) of a compound is defined as the sum of atomic weights of all atoms in the compound's molecule.

***Organics and Metals*** For most organics (except PCDDs and PCDFs) and metals, *MW* values were obtained from the following:

- Budavari, S., M.J. O'Neil, A. Smith, and P.E. Heckelman. 1989. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 11th Edition. Merck and Company, Inc. Rahway, New Jersey.

*MW* values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from the following document:

- Montgomery, J.H., and L.M. Welkom. 1991. *Groundwater Chemicals Desk Reference.* Lewis Publishers. Chelsea, Michigan.

Because Budavari, O'neil, Smith, and Heckelman (1989) provides *MW* values for most of the compounds evaluated, it was used as the primary source to ensure consistency. *MW* values are based on the compound's formula; and, the values in Budavari, O'Neil, Smith, and Heckelman (1989) are the same as the values cited in several literature sources. *MW* values for most of the compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

***PCDDs and PCDFs*** *MW* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a).

***Mercuric Compounds*** *MW* values for mercury and mercuric chloride were obtained from Budavari and others (1989). *MW* value for methyl mercury was obtained from U.S. EPA (1997g).

**Melting Point Temperature ($T_m$)**

Melting point temperature ($T_m$) is the temperature of the compound (in degree Kelvin [K]) at which the solid state of the compound undergoes a phase change to a liquid phase. At ambient temperatures and at an atmpospheric pressure of 1 atmosphere, compounds are either in a solid or liquid state.

***Organics and Metals*** For most organics (except PCDDs and PCDFs) and metals, values for $T_m$ were obtained from Budavari, O'Neil, Smith, and Heckelman (1989). $T_m$ values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from Montgomery and Welkolm (1991).

Because Budavari, O'Neil, Smith, and Heckelman (1989) provides $T_m$ values for most of the compounds evaluated, it was used as the primary source to ensure consistency. $T_m$ values in Budavari, O'Neil, Smith, and Heckelman (1989) were generally within 2 to 3 degrees of the values provided in literature sources reviewed. $T_m$ values for most compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

***PCDDs and PCDFs*** *Tm* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). U.S. EPA (1994a) provides $T_m$ values for PCDDs and PCDFs, that were obtained from various literature sources.

**Vapor Pressure (*Vp*) and Aqueous Solubility (*S*)**

The vapor pressure (*Vp*) of a substance is defined as the pressure in atmospheres exerted by the vapor (gas) of a compound when it is under equilibrium conditions. It provides a semi-quantitative rate at which it will volatilize from soil and/or water. The aqueous solubility (*S*) of a compound is defined as the saturated concentration of the compound in water (mg chemical/L water) at a given temperature and pressure, usually at soil/water temperatures and atmospheric pressure (Montgomery and Welkom 1991).

***Organics*** For most organics (except PCDDs and PCDFs), values for *Vp* and *S* were obtained from the following:

- U.S. EPA 1994b. *Draft Report Chemical Properties for Soil Screening Levels*. Prepared for the Office of Emergency and Remedial Response. Washington, DC. July 26.

U.S. EPA (1994b) provides measured, calculated, and estimated values for *Vp* and *S* that were obtained from various literature sources. *Vp* values in U.S. EPA (1994b) were generally either measured (at 20°C to 25°C) or calculated values obtained from various literature sources. U.S. EPA (1994b), however, provides values for *Vp* corrected to 25°C. U.S. EPA (1995a) states that, because the distribution of many of the parameters is skewed, the geometric mean or the median values were preferable to the arithmetic mean values. Therefore, when available geometric mean values were preferred over the arithmetic mean values.

In U.S. EPA (1994b), *S* values were either measured (at 20°C to 30°C) or calculated values obtained from various literature sources. Although *S* values were measured at temperatures ranging from 20°C to 30°C, U.S. EPA (1994b) states that *S* values were not corrected to 25°C, because the variability in solubilities measured at 20°C to 25°C was within the overall range of measured values.

U.S. EPA (1994b) is the preferred source, because (1) sources and the conditions at which each value was obtained are provided, and (2) values were provided to 2 significant figures. Also, U.S. EPA

(1994b) provides multiple *Vp* and *S* values for each compound from several different literature sources; providing a recent, more comprehensive compilation of reported literature values. *Vp* and *S* values from U.S. EPA (1994b) were generally consistent with those provided in U.S. EPA (1994e) and U.S. EPA (1995a).

When *Vp* and *S* values were not available in U.S. EPA (1994b), they were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994e)

2. U.S. EPA (1995a); values from which were obtained from one of three sources:

    a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II-Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

    b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

    c. Other referenced literature sources, when values were not available in Mackay, Shiu, and Ma (1992) or Howard (1989-1993).

3. U.S. EPA. 1994f. *Superfund Chemical Data Matrix (SCDM).* Office of Emergency and Remedial Response. Washington, DC. June.

*Vp* and *S* values in U.S. EPA (1994e) were geometric mean values obtained from various literature sources. References specific to sources of values for each compound were provided in U.S. EPA (1994e) and were, therefore, preferred over U.S. EPA (1995a) values.

Most *Vp* and *S* values in U.S. EPA (1995a) were obtained from Mackay, Shiu, and Ma (1992) or Howard (1989-1993). Mackay, Shiu, and Ma (1992) and Howard (1989-1993) obtain the "best" values after evaluation of various literature sources.

*Vp* values in U.S. EPA (1994f) were obtained from various literature sources. *S* values in U.S. EPA (1994f) were the geometric mean of values obtained from various literature sources.

***Mercuric Compounds*** Mercury is a relatively volatile compound. *Vp* and *S* values for elemental mercury were obtained from Budavari, O'Neil, Smith, and Heckelman (1989). *Vp* and *S* values for methyl mercury were not found in the literature.

**Henry's Law Constant (*H*)**

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentation of the compound in water at a given

temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure. Experimental and estimated *H* values from literature reports, however, are (1) very temperature-dependent and difficult to measure, (2) generally obtained from various literature sources that use different experimental and estimation methods, and (3) available for only a limited number of compounds.

***Organics*** For organics (excluding PCDDs and PCDFs), *H* values were calculated from the following theoretical equation (Lyman, Reehl, and Rosenblast 1982) for consistency, using recommended *MW, S,* and *Vp* values:

$$H = \frac{Vp \cdot MW}{S} \qquad \text{Equation A1-1}$$

| | | |
|---|---|---|
| *H* | = | Henry's Law constant (atm-m$^3$/mole) |
| *Vp* | = | Vapor pressure of Chemical (atm) |
| *S* | = | Solubility of Chemical in water (mg Chemical/L water) |

The primary guidance documents also used theoretical Equation A-1-1 to calculate *H* values.

***PCDDs and PCDFs*** *H* values for PCDDs and PCDFs are calculated values obtained from U.S. EPA (1994a).

***Metals*** For all metals (except mercury), *H* is zero, because *Vp*—because of the nonvolatile nature of the metals—and *S* are assumed to be zero.

***Mercuric Compounds*** *H* values for elemental mercury, and methyl mercury were obtained from U.S. EPA (1997g).

**Diffusivity of Chemicals in Air ($D_a$) and Water ($D_w$)**

Diffusivity or diffusion coefficients in air ($D_a$) and water ($D_w$) are used to calculate the liquid or gas phase transfer of a Chemical into a waterbody.

***Organics*** For organics (except PCDDs and PCDFs), diffusivity values were obtained directly from the CHEMDAT8 model chemical properties database (Worksheet DATATWO.WK1):

- U.S. EPA. 1994d. *CHEM8—Compound Properties Estimation and Data*. Version 1.00. CHEMDAT8 Air Emissions Program. Prepared for Chemicals and Petroleum Branch, OAQPS. Research Triangle Park. North Carolina. November 18.

The U.S. EPA (1994c) database uses empirical correlations with compound density and molecular weight to calculate diffusivity values. For compounds not in the U.S. EPA (1994c) database, diffusivity values were obtained by using the WATER8 model correlation equations for air and water diffusivities:

- U.S. EPA. 1995d. *WATER8—Air Emissions Models Wastewater Treatment*. Version 4.0. OAQPS. Research Triangle Park. North Carolina. May 1.

U.S. EPA(1995c) database values were predicted by using chemical-structural relationships. Diffusivity values for all compounds in the U.S. EPA (1994c) and (1995c) databases were either predicted or estimated. The primary guidance documents also recommended U.S. EPA (1994c) and (1995c) database model values. More recent documents, including the following, also recommended these values:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

For diffusivity values that were not available in these databases, $D_w$ and $D_a$ values were calculated using the following equations cited and recommended for use in U.S. EPA (1997g):

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}} \qquad \text{Equation A1-2a}$$

$$D_{w,i} = \frac{22\times10^{-5}}{(MW_i)^{2/3}} \qquad \text{Equation A1-2b}$$

U.S. EPA (1995a) recommended the use of standard default diffusivity values. U.S. EPA (1995a) stated that the diffusivity parameters vary slightly, and default values appear to be within the range of typical values. Values for diffusivity in air range from about 0.01 to 0.1 square centimeters per second ($cm^2/s$); therefore, U.S. EPA (1995a) recommended a default value of 0.08 $cm^2/s$. Values for diffusivity in water range from 1 x $10^{-06}$ to 1 x $10^{-05}$ $cm^2/s$; therefore, U.S. EPA (1995a) recommended a default value of 8 x $10^{-06}$ $cm^2/s$. Diffusivity values calculated using Equations A-1-2a and A-1-2b were within the range specified by U.S. EPA (1995a).

***PCDDs and PCDFs*** Diffusivity values in air and water for (1) 2,3,7,8-TCDD were obtained from U.S. EPA (1994c).

***Metals and Mercuric compounds*** For metals (except chromium and mercury), diffusivity values were not available in the literature. Diffusivity values for chromium and mercury were obtained from the U.S. EPA (1994c) database. The diffusivity value for methyl mercury was calculated using Equations A-1-2a and A-1-2b.

**Octanol/Water Partitioning Coefficient ($K_{ow}$)**

The *n*-octanol/water partitioning coefficient ($K_{ow}$) is defined as the ratio of the solute concentration in the water-saturated *n*-octanol phase to the solute concentration in the *n*-octanol-saturated water phase (Montgomery and Welkom 1991).

***Organics*** For organics (except PCDDs and PCDFs), $K_{ow}$ values were obtained from U.S. EPA (1994b). U.S. EPA (1994b) provides measured, calculated, and estimated $K_{ow}$ values obtained from various literature sources.

$K_{ow}$ values that were not available in U.S. EPA (1994b) were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994e)

2. Karickhoff, S.W. and J.M. Long. 1995. "Internal Report on Summary of Measured, Calculated, and Recommended Log $K_{ow}$ Values." Environmental Research Laboratory. Athens. April 10.

3. U.S. EPA (1995a), values from which were obtained from one of three sources:

   a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II - Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

   b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

   c. Other literature sources, when values were not available in Mackay, Shiu, and Ma (1992) and Howard (1989-1993).

***PCDDs and PCDFs*** $K_{ow}$ values for the PCDDs and PCDFs were obtained from either U.S. EPA (1994a) or U.S. EPA (1992a). U.S. EPA (1994a) and U.S. EPA (1992a) provide $K_{ow}$ values for PCDDs and PCDFs that were either measured values obtained from the literature or calculated by averaging the literature values within the homologue group. According to U.S. EPA (1994a), $K_{ow}$ values for hexachlorodibenzofurans were not available in the literature. Therefore, as recommended in U.S. EPA (1994a), due to lack of data, homologue group average values for hexachlorodibenzodioxins were applied to hexachlorodibenzofurans.

***Metals*** No $K_{ow}$ values were available for metals, either in the literature or in the primary guidance documents. $K_{ow}$ values for the metals were assumed to be zero, because the affinity of the metals to the octanol is almost zero.

***Mercuric compounds*** No $K_{ow}$ values were available in the literature for mercury and methyl mercury. For mercuric chloride, the $K_{ow}$ value was obtained from U.S. EPA (1997g).

**Soil Organic Carbon-Water Partition Coefficient ($K_{oc}$)**

The soil organic carbon-water partition coefficient ($K_{oc}$) or the organic carbon normalized soil sorption coefficient is defined as the ratio of adsorbed compound per unit weight of organic carbon to the aqueous solute concentration (Montgomery and Welkom 1991).

***Organics*** Because of the soil mechanisms that are inherently involved, $K_{oc}$ values for the ionizing organics and nonionizing organics are discussed separately.

**Ionizing Organic Compounds**

Ionizing organic compounds include amines, carboxylic acids, and phenols. These compounds contain the functional groups that ionize under specific pH conditions, and include the following:

- Organic acids (2,4,6-trichlorophenol; pentachlorophenol; 2,3,4,5-tetrachlorophenol; 2,3,4,6-tetrachlorophenol; 2,4,5-trichlorophenol; 2,4-dichlorophenol; 2-chlorophenol; phenol; 2,4-dimethylphenol; 2-methylphenol; 2,4-dinitrophenol; and benzoic acid)

- Organic bases—n-nitroso-di-n-propylamine; n-nitrosodiphenylamine, and 4-chloroaniline)

$K_{oc}$ values for ionizing organic compounds were obtained from U.S. EPA (1994b). U.S. EPA (1994b) provides $K_{oc}$ values for the ionizing organic compounds that have been estimated on the basis of the degree of ionization and the relative proportions of neutral and ionized species. The primary guidance documents cite one value for the ionizing organics, independent of the pH. The primary guidance documents calculate $K_{oc}$ values for the ionizing organics by using correlation equations containing $K_{ow}$ that are applicable to nonionizing organics. However, $K_{oc}$ values for ionizing compounds can vary vastly, depending on the pH conditions in the environment. For the ionizing organic compounds, the estimated $K_{oc}$ values based on pH are provided.

$K_{oc}$ values were estimated on the basis of the assumption that the sorption of ionizing organic compounds is similar to hydrophobic organic sorption, because the soil organic carbon is the dominant sorbent. According to U.S. EPA (1994b), for low pH conditions, these estimated values may overpredict sorption coefficients, because they ignore sorption to components other than organic carbon.

**Nonionizing Organic Compounds**

Nonionizing organic compounds are all other organic compounds not listed earlier as ionizing. They include volatile organics, chlorinated pesticides, polynuclear aromatic hydrocarbons (PAHs), and phthalates. The geometric mean of measured $K_{oc}$ values are provided in the following document:

- U.S. EPA. 1996a. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

U.S. EPA (1996a) calculated the geometric mean value from various measured values. For compounds for which $K_{oc}$ values are not provided by U.S. EPA (1996a), $K_{oc}$ values were calculated using $K_{ow}$ correlation equations provided in the same document.

***Metals*** For metals, no $K_{oc}$ values were found in the literature. For metals, soil/sediment-water partitioning coefficients (*Kd*) were obtained directly from experimental measurements.

**Chemical Partitioning, Partitioning Coefficients for Soil-Water ($Kd_s$) and Suspended Sediment-Surface Water ($Kd_{sw}$)**

Partition coefficients (*Kd*) describe the partitioning of a compound between sorbing material, such as soil, soil pore-water, surface water, suspended solids, and bed sediments. For organic compounds, *Kd*

has been estimated to be a function of the organic-carbon partition coefficient and the fraction of organic carbon in the partitioning media. For metals, *Kd* is assumed to be independent of the organic carbon in the partitioning media and, therefore, partitioning is similar in all sorbing media.

The soil-water partition coefficient ($Kd_s$) describes the partitioning of a compound between soil pore-water and soil particles, and strongly influences the release and movement of a compound into the subsurface soils and underlying aquifer. The suspended sediment-surface water partition coefficient ($Kd_{sw}$) coefficient describes the partitioning of a compound between surface water and suspended solids or sediments.

***Organics*** For organics (including PCDDs and PCDFs), soil organic carbon is assumed to be the dominant sorbing component in soils and sediments. Therefore, *Kd* values were calculated using the following fraction organic carbon ($f_{OC}$) correlation equations:

$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-1-3a}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-1-3b}$$

- U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA (1993d), from literature searches, states that $f_{OC}$ could range as follows:

- 0.002 to 0.024 in soils—for which a mid-range value of $f_{oc,s}$ = 0.01 generally can be used.
- 0.05 to 0.1 in suspended sediments—for which a mid-range value of $f_{oc,sw}$ = 0.075 generally can be used.

The DTSD uses mid-range $f_{oc}$ values recommended by U.S. EPA (1993). *Kd* values were calculated using $K_{oc}$ values recommended for each compound.

***Metals*** For metals (except mercury), *Kd* is governed by factors other than organic carbon, such as pH, redox, iron content, cation exchange capacity, and ion-chemistry. Therefore, *Kd* values for metals cannot be calculated using the same correlation equations specified for organic compounds. Instead, *Kd* values for the metals must be obtained directly from literature sources. *Kd* values for all metals, except lead, were obtained from U.S. EPA (1996a). U.S. EPA (1996a) provides values for *Kd* that are based on pH, and are estimated by using the MINTEQ2 model, which is a geochemical speciation model. The MINTEQ2 model analyses were conducted under a variety of geochemical conditions and metal concentrations. The MINTEQ2 pH-dependent *Kd* values were estimated by holding constant the iron oxide at a medium value and the $f_{oc}$ at 0.002. For arsenic, hexavalent chromium, selenium, and thallium, empirical pH-dependent *Kd* values were used.

*Kd* value for lead was obtained from the following:

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

***Mercuric Compounds*** Both watershed erosion and direct atmospheric deposition can be important sources of mercury to a water body (U.S. EPA 1997g). There appears to be a great deal of variability in the processing of mercury among water bodies. This variability is primarily a result of the characteristically wide range of chemical and physical properties of water bodies that influence the levels of methylated mercury. Some of the mercury entering the water body is methylated predominately through biotic processes (U.S. EPA 1997g). In the absence of modeling site-specific water body properties and biotic conditions, consistent with U.S. EPA (1997g), U.S. EPA OSW recommends 85 percent of total mercury in surface water is assumed to be divalent mercury and the remaining mass as methyl mercury. For the fish ingestion pathway, the DRAS converts the total mercury in the surface water to the methyl mercury fraction by multiplying the total mercury concentration in a second order stream by 0.15 to determine the methyl mercury concentration. $Kd_s$ values for mercury and methyl mercury were obtained from U.S. EPA (1996a). The *Kd* value for methyl mercury was obtained from U.S. EPA (1997g).

**Aquatic Toxicity Reference Values (*Aquatic TRVs*)**

Ecological benchmarks were developed for the protection of the aquatic community. These ecological benchmarks are referred to as toxicity reference values (TRVs) and were developed from a variety of ecological receptors based on the availability of data for a given waste constituent. The TRV is developed to protect the entire community, not one particular species. In general, TRVs (the measurement endpoints) were selected for consistency with the Agency's "Framework for Ecological Risk Assessment" (U.S. EPA 1992b). Region 6 believes the ecological analysis is conservative with respect to the overall assessment endpoint (e.g., sustainability of the reproducing populations) because of the way the source, fate and transport parameters are set and how the TRVs are developed.

The ecological assessment focused on inferring the sustainability of populations and communities within the aquatic ecosystem. Therefore, TRVs were derived from measurement endpoints (i.e., reproductive, developmental, growth, survival, and mortality) from which such inferences could be made. Reproductive studies (e.g., number of viable young per female) were preferred over other endpoints. The aquatic TRVs defaulted to a more conservative no effects level (or concentration) approach for ecological receptors. For populations of fish and aquatic invertebrates (represented by daphnids), a hierarchical approach was taken for use of data sources in deriving aquatic TRVs. The first choice was the final chronic values (FCVs) from the Ambient Water Quality Criteria (AWQC) effort by the EPA Office of Water (U.S. EPA 1998a). If these benchmarks were not available, then a freshwater aquatic TRV was selected from the draft *Protocol for Screening Level Ecological Risk Assessment at Hazardous Waste Combustion Facilities* (U.S. EPA. 1998b). Finally, TRVs were selected from the *Toxicological Benchmarks for Screening Potential contaminants of Concern for Effects on Aquatic Biota* (Suter and Tsao, 1996).

## A.1.3 BIOTRANSFER FACTORS FOR ANIMALS

### Bioconcentration and Bioaccumulation Factors for Chemicals in Fish

Bioconcentration and bioaccumulation factors for fish are used for various compounds, depending on the $K_{ow}$ value of the organic compound. Bioconcentration factors for fish ($BCF_{fish}$) were used for organics with a log $K_{ow}$ value less than 4.0; and for metals (except lead and mercury). Bioaccumulation factors for fish ($BAF_{fish}$) were used for organics with a log $K_{ow}$ value greater than 4.0, lead, and mercuric compounds.

### Bioconcentration Factors for Chemicals in Fish ($BCF_{fish}$)

$BCF_{fish}$ is the ratio of the chemical concentration in fish to the chemical concentration in the water column where the fish is exposed. It accounts for uptake of chemicals by fish from water passing across the gills. *BCF* values for fish were used for all organic compounds with a log $K_{ow}$ of less than 4.0 (cutoff value with $BAF_{fish}$) and for all metals, except lead and mercury, as cited in U.S. EPA (1995a). This implies that the concentration of chemical in the fish is only due to water intake by the fish, and compounds with a log $K_{ow}$ of less than 4.0 are assumed not to bioaccumulate.

BCF values reported in the DTSD Appendix are either:

1) Geometric mean of a valid number of field-measured values obtained from various field studies (or)
2) Geometric mean of laboratory-measured values obtained from various experimental studies (or)
3) Estimated values calculated using a correlation equation

**NOTE**: When only one valid field-measured value for a chemical was found in the literature, the higher of the field-measured value and the geometric mean of laboratory-measured values, was used.

In general, field measured BCFs were assumed to be based on total (dissolved and suspended) water column concentrations; and laboratory measured BCFs were assumed to be based on dissolved water column concentrations. This distinction is important for compounds with a log $K_{ow}$ of greater than or equal to 4.0, because significant amounts of a chemical can partition into the suspended sediment organic carbon (or particulate phase) of the water column. For compounds with a log $K_{ow}$ of less than 4.0, most of chemical is associated with the dissolved phase of the water column and negligible amounts of chemical is associated with the suspended sediment phase in the water column. Therefore, for compounds with a log $K_{ow}$ of less than 4.0, BCF values based on dissolved chemical water concentrations in the water column are essentially the same as BCF values based on total (dissolved + suspended) chemical water concentrations in the water column.

The DTSD does not recognize differences in total versus dissolved water concentrations when calculating fish concentrations from $BCF_{fish}$ values for compounds with a log $K_{ow}$ of less than 4.0. Since, dissolved water concentrations is the major contributing factor from compounds with a log $K_{ow}$ of less than 4.0, all $BCF_{fish}$ values (irrespective of whether they were derived using total or dissolved water concentrations) can be multiplied by chemical concentration in the dissolved water column ($C_{dw}$) to calculate fish concentrations. This assumption is necessary because (1) literature data is often unclear if the water concentrations are dissolved or total concentrations, and (2) most of the literature reviewed

indicated that laboratory experiments were conducted using filtered or distilled water; or the experiments were conducted using fresh water, but were filtered before analyses for water concentrations.

***Organics*** For organics with a log $K_{ow}$ value of less than 4.0, $BCF_{fish}$ values were obtained from either of two methods:

- Field-measured or laboratory-measured values from various experimental studies were evaluated by U.S. EPA (1998b). This information is summarized in the following document:

  U.S. EPA. 1998b. *Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities.* Draft Interim Final. April.

  Field-measured data is only (1) available for a limited number of compounds, and (2) based on a single study. In such cases, the field-measured value or the geometric mean of field-measured values were compared with the geometric mean of laboratory-measured values, and the higher one used. A detailed discussion on sources of BCF values and methodology followed are provided in Appendix C of U.S. EPA (1998b).

- When measured values were not available or could not be evaluated, the following correlation equation recommended by Lyman, Reehl, and Rosenblatt (1982) was used:

$$\log BCF_{fish} = -0.23 + 0.76 \log K_{ow} \qquad \text{Equation A-1-4}$$

Correlation Equation A-1-4 was developed by the following:

- 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." *Journal of Fish. Res. Board Can.* Prepublication Copy.

Veith, Macek, Petrocelli, and Caroll (1980) measured *BCF* values for four fish species in flow-through laboratory studies that were exposed to a wide range of organic chemicals. $BCF_{fish}$ values calculated by using correlation Equation A-1-4 are (1) based on dissolved water concentrations, and (2) not lipid-normalized.

***Metals*** For metals (except lead and mercury), $BCF_{fish}$ values are measured values obtained from various literature studies, as cited in U.S. EPA (1998b). Measured values from various experimental studies were evaluated by U.S. EPA (1998b). Detailed discussion and sources of measured values were provided in U.S. EPA (1998b). For lead, a BAF is more applicable than a BCF as it tends to bioaccumulate.

***Mercuric Compounds*** For mercuric compounds, a BAF is more applicable than a BCF as they tend to bioaccumulate. Therefore the $BAF_{fish}$ value for methyl mercury was obtained from U.S. EPA (1997g) for a trophic level 4 fish.

**Bioaccumulation Factors for Chemicals in Fish ($BAF_{fish}$)**

$BAF_{fish}$ is the ratio of the chemical concentration in fish to the chemical concentration in the water body where the fish are exposed. The $BAF_{fish}$ accounts for uptake of chemicals by fish from water and sediments passing across the gills, and from consumption of various foods including plankton, daphnids, and other fish. BAFs for fish were used for organic compounds (except PCBs, PCDDs, and PCDFs) with a log $K_{ow}$ greater than 4.0, lead and mercuric compounds.

For compounds with a log $K_{ow}$ of greater than or equal to 4.0, chemicals can significantly partition into the suspended sediment organic carbon (or particulate phase) of the water column. Therefore, BAF values should be based on total (dissolved and suspended) water column concentrations. BAFs reported are either:

1) Geometric mean of field-measured values obtained from various experimental studies (or)
2) Predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured BCFs. A FCM is the ratio of a BAF to a BCF, and is used to account for food chain biomagnification from a lower to a upper trophic level (or)
3) Predicted values calculated by multiplying a FCM with an estimated BCF. BCFs were estimated using correlation Equation A-1-4.

**NOTE**: When only one valid field-measured value for a chemical was found in the literature, the higher of the field-measured value and the geometric mean of laboratory-measured values, was used.

In general, (1) field-measured BAFs were assumed to be based on total (dissolved and suspended) water column concentrations, (2) laboratory-measured BCFs, and therefore, the BAFs predicted from them, were assumed to be based on dissolved water column concentrations, and (3) estimated BCFs using correlation Equation A-1-4, and therefore, the BAFs predicted from them, were assumed to be based on dissolved water column concentrations. In addition, field-measured BCFs, for compounds with a log $K_{ow}$ greater than 4.0, were assumed to be equal to BAFs, because the tissue concentrations are a result of uptake of water (dissolved and suspended), sediment, and various trophic level food.

For consistency, all field-measured BAF (or BCF) values were adjusted according to the methodology specified in U.S. EPA (1995e) to include only the dissolved water column fractions; (i.e., the BAFs based on total water concentrations were converted to BAFs based on dissolved water concentrations). This was done, so that all $BAF_{fish}$ values (based on dissolved water concentrations) can be multiplied by the chemical concentration in the dissolved water column ($C_{dw}$) to calculate fish concentrations.

In U.S. EPA (1995a), BAF values were estimated based on the models developed for the limnetic ecosystem by the following:

- Thomann, R.V. 1989. "Bioaccumulation Model of Organic Chemical Distribution in Aquatic Food Chains." *Environmental Science and Technology*. 23(6):699-707.

and, for the littoral ecosystem by the following:

- Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992. "An Equilibrium Model of Organic Chemical Accumulation in Aquatic Food Webs with Sediment Interaction." *Environmental Toxicology and Chemistry.* 11:615-629.

BAF values were predicted by multiplying a laboratory-measured or predicted BCF by a FCM. The Thomann (1989) and Thomann, Connolly, and Parkerton (1992) models were adopted by U.S. EPA, Office of Water, for the Great Lakes Water Quality Initiative in 1993. In 1995, U.S. EPA, Office of Water, developed BAFs based on the following study:

- Gobas, F.A.P.C. 1993. "A Model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario." Ecological Modelling. 69:1-17.

The Gobas (1993) model was adopted to develop the latest water quality criteria and is provided in the following two documents:

- U.S. EPA. 1995d. *Water Quality Guidance for the Great Lakes System. Supplementary Information Document.* Office of Water. EPA-820-B-95-001. March.

- U.S. EPA. 1995e. *Great Lakes Water Quality Initiative. Technical Support Document for the Procedure to Determine Bioaccumulation Factors*. Office of Water. EPA-820-B-95-005. March.

The Gobas (1993) food-chain model was preferred because, unlike the Thomann (1989) model, it includes both benthic and pelagic food chains, thereby estimating exposure of organisms to compounds from both the sediment and the water column. Other inherent drawbacks of the Thomann (1989) model were that the model: (1) did not take into account metabolism, biotransformation, degradation, persistence, or seasonal or temporal variability, (2) is extremely sensitive to certain input parameter such as the lipid content, (3) incorrectly adopted FCMs, (4) is questionable in its assumption that the system is at steady state or in equilibrium, and (5) had little application for compounds with a log $K_{ow}$ greater than 6.5, because the sediment route of exposure was not considered.

The Gobas (1993) model: (1) accounts for metabolism, but sets the metabolic rate to zero because of lack of data for individual compounds, (i.e., the metabolism is assumed not to occur), (2) incorporates the concentration of the compound in both the sediment and the water column, the sediment route being especially useful for compounds with a log $K_{ow}$ greater than 6.5, and (3) includes the disequilibrium between concentrations of the compounds in sediment and the water column. Although the Thomann, Connolly, and Parkerton (1992) model accounts for sediment interaction, according to U.S. EPA (1995d), the Gobas (1993) model required fewer input parameters which could be more easily specified.

The following equation cited in U.S. EPA (1995e) was used to convert the BAF based on total water concentrations to a BAF based on dissolved water concentrations:

$$f_{fd} = \frac{1}{1 + \frac{(DOC)\ (K_{ow})}{10} + (POC)\ (K_{ow})} \qquad \text{Equation A-1-5}$$

where

$f_{fd}$ = fraction of chemical that is freely dissolved in water
$DOC$ = concentration of dissolved organic carbon, kg organic carbon / L water
$POC$ = concentration of particulate organic carbon, kg organic carbon / L water

Since, the Gobas (1993) model was derived from a study conducted at Lake Ontario, DOC and POC values for Lake Ontario were used. Values cited in U.S. EPA (1995e) were:

DOC = $2 \times 10^{-6}$ kg/L
POC = $7.5 \times 10^{-9}$ kg/L

A BAF based on dissolved water concentrations can be calculated from a BAF based on total water concentrations as follows:

$$BAF\ (dissolved) = \frac{BAF\ (total)}{f_{fd}} - 1 \qquad \text{Equation A-1-6}$$

FCMs were obtained from Table 2 of U.S. EPA (1995e). U.S. EPA (1995e) provided FCMs as a function of log $K_{ow}$ in increments of 0.1 for trophic level 2, 3, and 4 aquatic organisms. Humans are assumed to consume trophic level 3 or 4 fish. The higher FCM value of trophic levels 3 and 4 was used. When the log $K_{ow}$ value of a chemical was between two log $K_{ow}$ values listed in Table 2 of U.S. EPA (1995e), the FCM for the next highest log $K_{ow}$ value was used.

***Organics*** For all organics (except PCBs, PCDDs and PCDFs) with a log $K_{ow}$ greater than or equal to 4.0, the FCM, which accounts for accumulation through the food chain in addition to water, becomes greater than 1. Therefore, a $BAF_{fish}$, which takes the food chain into consideration, is more appropriate than a $BCF_{fish}$.

For all organics with a log $K_{ow}$ greater than or equal to 4.0, BAFs were derived using one of following three methods:

1) BAF = Field measured BAF or BCF, adjusted for dissolved water concentrations
2) BAF = Laboratory measured BCF multiplied by a FCM for either trophic level 3 or 4 fish
3) BAF = Estimated BCF calculated using correlation equation A-1-4 multiplied by a FCM for either trophic level 3 or 4 fish

Both field and laboratory measured values were derived from various literature sources cited in U.S. EPA (1998b). FCMs were obtained from U.S. EPA (1995e).

***Metals (lead)*** For lead, the food-chain multiplier becomes greater than 1; therefore, a BAF is more appropriate. The $BAF_{fish}$ value for lead was obtained as a geometric mean from various literature sources described in U.S. EPA (1998b). Since metals are assumed insoluble under neutral conditions, the dissolved and total water concentrations are almost equal. However, for consistency, the $BAF_{fish}$ value for lead was adjusted for dissolved fractions.

***Mercuric Compounds*** For mercuric compounds, a BAF is more applicable than a BCF as they tend to bioaccumulate. Therefore the $BAF_{fish}$ value for methyl mercury was obtained from U.S. EPA (1997g) for a trophic level 4 fish.

## A.1.4 HUMAN HEALTH BENCHMARKS

### Reference Dose (*Rfd*) and Reference Concentration (*RfC*)

Reference dose (*Rfd*) is defined as a daily intake rate of a compound estimated to pose no appreciable risk of deleterious effects over a specific exposure duration (U.S. EPA 1989). Reference concentration (*Rfc*) is defined as the concentration of a compound estimated (with uncertainty spanning perhaps an order of magnitude) to pose no appreciable risk of deleterious effects over a specific exposure duration (U.S. EPA 1989).

The reference dose (*RfD*) and reference concentration (*RfC*) values for all compounds were obtained from one of the following references (listed in order of preference):

- U.S. EPA. 1997b. *Integrated Risk Information System (IRIS).* June - December.
- U.S. EPA. 1995b. "Health Effects Assessment Summary Tables (HEAST)." Fiscal Year Annual 1995. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/036.
- U.S. EPA. 1997c. "Health Effects Assessment Summary Tables (HEAST)." Fiscal Year Annual 1997. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/036.
- U.S. EPA. 1997d,e,f. " Risk Assessment Issue Papers". Superfund Technical Support Center. National Center for Environmental Assessement. December.
- U.S. EPA. 1997a. "Risk-Based Concentrations." Region 3. June
- U.S. EPA. 1996b. "Region 9 Preliminary Remediation Goals." Region 9. August.

The U.S. EPA (1997b) IRIS database and the U.S. EPA (1995b, 1997c) HEAST are compilations of human health risk information obtained from several literature sources. U.S. EPA (1995b, 1997c) cited IRIS as the main source of human health risk information.

*RfD* and *RfC* values were revised as values in U.S. EPA (1997b) and U.S. EPA (1995b, 1997c) are updated regularly.

### Oral Cancer Slope Factor (CSF), Inhalation CSF, and Inhalation Unit Risk Factor (URF)

*Oral CSF*, *inhalation CSF*, and *inhalation URF* values for all compounds were obtained from U.S. EPA (1997b) or (1995b, 1997c). In addition, U.S. EPA (1996b; 1997a,d,e,f) were also used to obtained the *oral CSF*, *inhalation CSF*, and the *inhalation URF* when these values were not available in U.S. EPA (1997b) or (1995b; 1997c). Additional guidance for determining reference concentrations for chronic inhalation exposure is provided in U.S. EPA (1994h).

**Explanation of Calculated Toxicity Benchmark Values**

The preference for health benchmarks is to obtain values from IRIS or HEAST. The following methodology was used to calculate missing benchmarks using available benchmarks that are based on route-to-route extrapolation:

1) *Oral RfD*s presented in IRIS/Heast/EPA reviewed documents were used if available. Missing oral *RfD*s were calculated from the *RfC* assuming route-to-route extrapolation using the following equation:

$$Oral\ RfD = \frac{RfC \cdot 20\ m^3/d}{70\ kg\ BW} \qquad \text{Equation A1-7}$$

2) *Oral CSF*s presented in IRIS/Heast/EPA reviewed documents were used when available. In the case of missing Oral CSFs:

   a) *Oral CSF = Inhalation CSF*, or

   b) *Oral CSF = Inhalation CSF* calculated from Inhalation URF assuming route-to-route extrapolation.

3) *Inhalation RfC*s presented in IRIS/Heast/EPA reviewed documents were used when available. If *RfC*s were not available they were calculated from the *RfD* assuming route-to-route extrapolation using the following equation:

$$Inhalation\ RfC = \frac{RfD \cdot 70\ kg\ BW}{20\ m^3/d} \qquad \text{Equation A1-8}$$

4) *Inhalation* $RfD_i$ values were calculated as follows:

   a) From the *inhalation RfC* obtained from IRIS/Heast/EPA reviewed documents using the following equation:

$$RfD_i = \frac{RfC \cdot 20\ m^3/d}{70\ kg} \qquad \text{Equation A1-9}$$

   b) If the *RfC* was not available from IRIS/Heast/EPA reviewed documents, the following was assumed:

$$Inhalation\ RfD = Oral\ RfD$$

5) For *inhalation URF*s, values were obtained from IRIS/Heast/EPA reviewed documents. If the *inhalation URF*s were not available they were calculated from *oral CSF*, using the following equation:

$$Inhal.\ URF = \frac{Oral\ CSF \cdot 20\ m^3/d}{70\ kg \times 1000\ \mu g/mg} \qquad \text{Equation A1-10}$$

6) The *inhalation CSF*s presented in IRIS/Heast/EPA reviewed documents were used when available.

   a) If no *inhalation CSF* was available; it was calculated from *inhalation URF*, using the following equation:

$$Inhal.\ CSF = \frac{Inhal.\ URF \cdot 70\ kg}{20\ m^3/d} \times 1000\ \mu g/mg \qquad \text{Equation A1-11}$$

   b) If no *inhalation URF* was available; the following was assumed based on route-to-route extrapolation:

$$Inhalation\ CSF = Oral\ CSF$$

**Uncertainties Involved when using Toxicity Benchmarks Calculated based on Route-to-Route Extrapolation**

In the assessment of noncarcinogenic and carcinogenic risk from chemicals, EPA-derived or reviewed health benchmarks (*RfD*s, *RfC*s, *CSF*s, *URF*s, and *Inhalation CSF*s) are recommended. However, for numerous compounds, a complete set of inhalation and oral EPA-derived health benchmarks are not available. In such cases, the health benchmarks were calculated based on available EPA-derived benchmarks values. For instance, if the *oral RfD* (mg/kg/day) was available and the *RfC* (mg/m$^3$) was not; the *RfC* was calculated by multiplying the *RfD* by an average human inhalation rate of 20 m$^3$/day and dividing by the average human body weight of 70 kg. This conversion is based on a route-to-route extrapolation, which assumes that the toxicity of the given chemical is equivalent over all routes of exposure.

This process does introduce uncertainty into the risk assessment. By using this method, the risk assessor must assume that the qualitative data supporting the benchmark value for a certain route also applies to the route in question. For example, if an *RfD* is available and the *RfC* is calculated from that value, the risk assessor is assuming that the toxicity seen following oral exposure will be equivalent to toxicity following inhalation exposure. This assumption could overestimate or underestimate the toxicity of the given chemical following inhalation exposure.

Because of the degree of uncertainty involved in using toxicity benchmark values calculated based on route-to-route extrapolation, the DRAS recommends that a qualitative assessment of the toxicity information available for the chemical and exposure route be performed. This will enable the risk assessor to make a well informed decision concerning the validity of values calculated based on route-to-route extrapolation. This qualitative assessment should also be included in the uncertainty section of the risk assessment.

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# TABLE A-1a-1

# CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 154.21 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 368.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 4.93E-06 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.80E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.00E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.21E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.19E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 9.22E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 4.90E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.90E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.67E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.3E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 7.60E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.00E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.30E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.07E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-1

## CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.10E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 17 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-2

# CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 58.08 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 179.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.99E-01 at 25°C (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 6.04E+05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.88E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.87E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.15E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1998c). | 6.00E-01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.51E-01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.51E-03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.13E-02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.70E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.70E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.80E-05 |

## TABLE A-1a-2

## CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 4.00E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 1.5E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-3

# CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 41.05 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 318.1 |
| *Vp* (atm) | Howard (1989-1993) | 1.20E-01 at 25°C (solid) |
| *S* (mg/L) | Howard (1989-1993) | 1.30E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.79E+01 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.14E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.40E-05 |
| $K_{ow}$ (unitless) | log $K_{ow}$ value cited in Karickhoff and Long (1995). | 4.57E-01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 7.69E-01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.69E-03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.76E-02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.10E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.60E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.70E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.60E-05 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.25E-01 |

## TABLE A-1a-3

## CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.10E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-4

# CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 120.50 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 293.6 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 5.20E-04 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 6.10E+03 |
| *H* (atm·m$^3$/mol) | H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.03E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.00E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.73E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 4.37E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.69E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.69E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.02E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.10E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.40E-03 |

## TABLE A-1a-4

## CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.04E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *Oral RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data availabe

# TABLE A-1a-5

# CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 56.06 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 185.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 3.50E-01 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 2.10E+05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 9.34E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.92E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.22E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 9.80E-01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.39E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.39E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.05E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.50E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.60E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 9.80E-05 |

## TABLE A-1a-5

## CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.80E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 2.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997) | 2.0E-05 |
| *Inhalation URF* $(\mu g/m^3)^{-1}$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.1E+00 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-6

# CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 53.06 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 189.6 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) . | 1.40E-01 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) . | 7.50E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 9.90E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.11E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.23E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.78E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.22E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.22E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.66E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.43E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.80E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.40E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.80E-04 |

## TABLE A-1a-6

## CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 4.80E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 1.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 5.4E-01 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 2.0E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 2.4E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 7.6E+01 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-7

# CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 364.93 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 377.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1994b). | 2.20E-08 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1994b). | 7.84E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.35E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.43E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.40E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994f). | 1.51E+06 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 4.87E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.87E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.65E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.70E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.50E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.90E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.20E+02 |

# TABLE A-1a-7

## CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAF*s were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 5.82E+05 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.00E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.70E+01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.10E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.70E+01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3E-01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-8

# CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 93.12 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 266.8 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 8.80E-04 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 3.60E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 2.28E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.56E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.01E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 9.55E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.23E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.23E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.17E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.60E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.80E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 9.50E-04 |

## TABLE A-1a-8

## CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.27E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1996d) | 2.9E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 5.7E-03 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 1.0E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on Oral CSF assuming route-to-route extrapolation. | 5.7E-03 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-9

# CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 178.22 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 491.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 3.35E-08 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 5.37E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.11E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.24E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.74E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 2.95E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.35E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.35E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.76E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.61E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.07E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.50E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.47E+00 |

# TABLE A-1a-9

## CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 2.60E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 7.3E-01 |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-10

## CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 121.75 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 903.1 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | NA |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.73E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.96E-06 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 45 at pH=6.8 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 45 at pH=6.8 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995g) | 4.00E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-10

## CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1995d) | 4.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.43E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 6E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.60E+2 |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-11

## CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 74.92 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 1,091 at 36 atm |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.07E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.24E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 25 at pH=4.9;<br>29 at pH=6.8;<br>31 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 25 at pH=4.9;<br>29 at pH=6.8;<br>31 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.00E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | ND |
| *t** | t* value was obtained from U.S. EPA (1992b). | ND |
| *B* | *B* value was obtained from U.S. EPA (1992b). | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995g) | 2.00E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-11

## CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 3.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.5E+00 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1996d) | 1.5E+01 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-02 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 1.50E+02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-12

## CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 137.33 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 983 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.14E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.26E-06 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 11 at pH=4.9;<br>41 at pH=6.8;<br>52 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 11 at pH=4.9;<br>41 at pH=6.8;<br>52 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-12

## CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 7.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 5.0E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 2 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 3.9E+00 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-13

## CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 78.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 278.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.25E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.78E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.49E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.17E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.02E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 137 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 6.20E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.20E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.65E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.10E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.60E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.30E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.48E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-13

## CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | Calculated from the *RfC* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.70E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 2.90E-02 |
| *RfC* ($mg/m^3$) | U.S. EPA (1997e) | 6.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 2.90E-02 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 4.6E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-14

# CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 228.28 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 433 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.03E-10 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.28E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 3.62E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 2.47E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 6.21E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 4.77E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 2.60E+05 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.60E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.94E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.60E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.20E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.00E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 5.10E+03 |

## TABLE A-1a-14

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(a)anthracene of 0.1 (U.S. EPA 1993e) | 7.31E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.31E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 2.7E-02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-15

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 252.3 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 452 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 6.43E-12 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.94E-03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table. | 8.36E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d). | 2.18E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d). | 5.85E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.35E+06 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 9.69E+05 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.69E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.27E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.40E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 9.95E+03 |

## TABLE A-1a-15

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 7.30E+00 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.30E+00 |
| *MCL* | National Primary Drinking Water Regulations. | 2E-04 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.4E-02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-16

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 252.32 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 441 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 1.06E-10 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 4.33E-03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 6.18E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 2.28E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 5.49E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.59E+06 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.36E+05 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.36E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.27E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.40E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.60E+02 |

## TABLE A-1a-16

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 9.95E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.1 (U.S. EPA 1993e). | 7.3E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.3E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-17

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 252.32 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 490 |
| *Vp* (atm) | U.S. EPA (1994b) | 1.32E-12 at 25ºC (solid) |
| *S* (mg/L) | U.S. EPA (1994b) | 8.0E-04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 4.15E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 2.28E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 5.49E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 1.56E+06 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.32E-05 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.32E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.24E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.03E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.43E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E+02 |

## TABLE A-1a-17

## CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 9.95E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for benzo(k)fluoranthene of 0.01 (U.S. EPA 1993?) | 7.3E-02 |
| *RfC* ($mg/m^3$) | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.3E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-18

# CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 108.13 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 288.29 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.40E-04 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 4.00E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.78E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.89E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.38E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g). | 1.26E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.02E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.02E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.65E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 2.60E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.60E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.04E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-18

## CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.10 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 3.75E+02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-19

## CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 126.58 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 225.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.60E-03 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 4.90E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.13E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.43E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.80E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 2.00E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.83E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.83E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.62E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.40E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.00E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.11E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-19

## CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.70E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 1.70E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-20

# CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 9.01 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 1,560 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 4.39E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 5.08E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.20E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-20

## CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | | 8.4E+00 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 2.0E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 8.4E+00 |
| *MCL* | National Primary Drinking Water Regulations. | 4E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 5.1E+00 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-21

## CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 143.02 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 223.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 1.76E-03 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.18E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.13E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.40E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.70E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 2.00E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 7.60E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.60E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.70E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.80E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.50E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.60E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.60E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.74E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-21

## CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.1E+00 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.1E+00 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.380E+03 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-22

# CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 163.83 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 218.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 7.68E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.97E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.17E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.98E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.06E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.06E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.38E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.38E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.03E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 5.90E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.10E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.04E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-22

## CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 6.20E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 6.20E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-23

## CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (TRIBROMOMETHANE) (75-25-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 252.77 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 280.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 7.82E-03 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.21E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.16E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.41E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.03E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.24E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.26E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.26E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.45E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.609E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.20E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.60E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-23

## CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (TRIBROMOMETHANE) (75-25-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 7.90E-03 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 3.90E-03 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.93E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-24

# CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 249.2 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 291.8 |
| *Vp* (atm) | *Vp* value cited in Montgomery and Welkom (1991). | 1.97E-06 at 25ºC (liquid) |
| *S* (mg/L) | -- | ND |
| *H* (atm·m$^3$/mol) | -- | ND |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.98E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.83E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.10E+05 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.21E+05 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.21E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.09E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.30E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.89E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.63E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.91E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (unitless FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 1.46E+04 |

## TABLE A-1a-24

## CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 5.80E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.03E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.5E+00 |

Note:NA = Not applicable, ND = No data available

## TABLE A-1a-25

## CHEMICAL-SPECIFIC INPUTS FOR BUTYL-BENZYL PHTHALATE (85-68-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Howard (1989-1993) | 312.39 |
| $T_m$ (K) | Howard (1989-1993) | 238.0 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.58E-08 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.58E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.91E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.65E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.17E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.59E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.37E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.37E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.03E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 6.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 7.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.40E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.90E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 2.35E+03 |

## TABLE A-1a-25

## CHEMICAL-SPECIFIC INPUTS FOR BUTYL-BENZYL PHTHALATE (85-68-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.9E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-26

# CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 112.41 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 594.1 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.16E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 9.45E-06 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | Geometric mean value obtained from various literature sources (see Appendix A3.4). | 2.50E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-26

## CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD (water)* (mg/kg/day) | U.S. EPA (1997b) | 5.0E-04 |
| *RfD (food)* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 6.3E+00 |
| *RfC* ($mg/m^3$) | Calculated from *RfD (food)* value using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.5E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 6.3E+00 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 2.2E+00 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-27

# CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 76.14 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 161.5 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 4.47E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.67E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.27E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.04E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.29E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.00E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.14E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.14E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.86E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.50E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.10E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.95E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-27

## CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 7.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 1E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-28

# CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 153.84 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 250.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.48E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.92E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S*, and *Vp* values that are provided in this table. | 2.87E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.56E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.77E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.21E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 1.52E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.52E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.14E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.90E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 7.60E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.80E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.40E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 3.00E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-28

## CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 7.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.30E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.50E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 5.30E-02 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.52E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-29

# CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 409.80 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 381.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 3.55E-08 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 5.51E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.64E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.18E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.37E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 8.66E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 5.13E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.13E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.85E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.90E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.80E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+02 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.10E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.07E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-29

## CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 3.50E-01 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 7.00E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 3.50E-01 |
| *MCL* | National Primary Drinking Water Regulations. | 2E-03 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 4.3E--03 |

Note:NA = Not applicable, ND = No data available

## TABLE A-1a-30

## CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 71.90 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 172.1 |
| *Vp* (atm) | -- | ND |
| *S* (mg/L) | -- | ND |
| *H* (atm·m$^3$/mol) | -- | ND |
| $D_a$ (cm$^2$/s) | -- | 1.10E-01 |
| $D_w$ (cm$^2$/s) | -- | 1.27E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | -- | ND |
| $Kd_{sw}$ (L/Kg) | -- | ND |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | ND |
| *t* | *t* value was obtained from U.S. EPA (1992b). | ND |
| *t** | t* value was obtained from U.S. EPA (1992b). | ND |
| *B* | *B* value was obtained from U.S. EPA (1992b). | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-30

## CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA 1994e or U.S. EPA 1995c | 1.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 2.0E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: Not applicable, ND = No data available

## TABLE A-1a-31

## CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 142.58 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 328.6 |
| *Vp* (atm) | U.S. EPA (1998c) | 1.08E-05 |
| *S* (mg/L) | U.S. EPA (1998c) | 3.85E+03 |
| *H* (atm·m$^3$/mol) | U.S. EPA (1998c) | 4.00E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 6.96E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.06E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.26E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.71E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.71E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.78E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.09E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.50E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | ND |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.26E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.34E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-31

## CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-32

# CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 127.57 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 345.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 3.09E-05 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.36E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.17E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.80E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.02E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 7.40E+01 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | $K_{oc}$ is 41 for pH range of 4.9 to 8 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.06E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.05E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.50E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.10E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.55E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-32

## CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 4.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.40E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note:NA= Not applicable, ND= No data available

## TABLE A-1a-33

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 112.56 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 228.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.59E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 4.09E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.38E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.35E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.49E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 6.16E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.24E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.24E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.68E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.20E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.20E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 7.76E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-33

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 6.0E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 1E-01 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.3E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-34

# CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 325.20 |
| $T_m$ (K) | Howard (1989-1993) | 309.0 |
| *Vp* (atm) | Howard (1989-1993) | 2.90E-09 at 25ºC (solid) |
| *S* (mg/L) | Howard (1989-1993) | 1.30E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.24E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 1.65E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 4.72E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 2.40E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.69E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.69E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.77E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 2.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.50E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.40E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 2.03E+03 |

## TABLE A-1a-34

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 2.7E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 2.7E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-35

# CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Howard 1989-1993 | 86.47 |
| $T_m$ (K) | Howard 1989-1993 | 126.6 |
| *Vp* (atm) | *Vp* value cited in Howard 1989-1993. | 5.63E+00 at 25°C (liquid) |
| *S* (mg/L) | Howard 1989-1993 | 2.90E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.68E-01 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 9.72E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.13E-05 |
| $K_{ow}$ (unitless) | Calculated using the log $K_{ow}$ value cited in Howard 1989-1993. | 1.20E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.83E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.83E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.40E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | ND |
| *t* | *t* value was obtained from U.S. EPA (1992b). | ND |
| *t** | t* value was obtained from U.S. EPA (1992b). | ND |
| *B* | *B* value was obtained from U.S. EPA (1992b). | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.89E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-35

## CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmark** | | |
| *RfD* (mg/kg/day) | Calculated from *RfC* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.40E+01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | | ND |
| *RfC* ($mg/m^3$) | U.S. EPA (1997b) | 5.00+01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-36

# CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 64.52 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 441.8 |
| *Vp* (atm) | *Vp* value cited in Lucius et al. (1992). | 1.60E+02 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1994a) | 5.74E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.80 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.27E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.53E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value calculated from log $K_{ow}$ value cited in U.S. EPA (1995a). | 1.26E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.71E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.71E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.78E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.34E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-36

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 4.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 1.00E+01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-37

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (TRICHLOROMETHANE) (67-66-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 119.39 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 209.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.69E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.96E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.03E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.17E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.09E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 8.90E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 5.30E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.30E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.98E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.30E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.30E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 3.59E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-37

## CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (TRICHLOROMETHANE) (67-66-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 6.10E-03 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.0E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 8.10E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.89+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-38

## CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 171.07 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 369.9 |
| *Vp* (atm) | Montgomery and Welkom (1991) | 7.00E-03 at 25ºC (solid) |
| *S* (mg/L) | Montgomery and Welkom (1991) | 1.70E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.04E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.61E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.38E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in Howard (1989 - 1993). | 3.80E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.46E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.46E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.46E-02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.02E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.80E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.38E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-38

## CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 4.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | 1.4E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | ND |
| *Inhalation* [1] *CSF* $(mg/kg/day)^{-}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-39

# CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 162.61 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 332.6 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.05E-05 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.20E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.43E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.64E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.24E-06 |
| $K_{ow}$ (unitless) | Montgomery and Welkom (1991) | 1.17E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 7.14E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.14E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.86E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.63E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.59E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.84E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.32E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 9.60E+02 |

## TABLE A-1a-39

## CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 8.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.80E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-40

# CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 128.56 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 282.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.77E-03<br>at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.15E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.66E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.01E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.46E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.45E+02 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1-4 398.0<br>5 397.9<br>6 396.9<br>7 387.3<br>8 311.8<br>9 108.7<br>10 19.43<br>11 7.39<br>12 6.14<br>13 6.01<br>14 6.00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0. | 3.87E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.90E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.10E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.40E-02 |

## TABLE A-1a-40

## CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.59E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 4.4E+01 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-41

## CHEMICAL-SPECIFIC INPUTS FOR 4-CHLOROPHENYL-PHENYLETHER (7005-72-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 204.66 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 265.1 |
| *Vp* (atm) | *Vp* value cited in Montgomery and Welkom (1991). | 3.55E-06 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in Montgomery and Welkom (1991). | 3.30E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.20E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 3.82E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 4.42E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 5.85E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 7.40E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.40E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.55E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |

## TABLE A-1a-41

## CHEMICAL-SPECIFIC INPUTS FOR 4-CHLOROPHENYL-PHENYLETHER (7005-72-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 6.06E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-42

# CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 52 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 2,173.1 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database in U.S. EPA (1994f). | 1.01E-01 |
| $D_w$ (cm$^2$/s) | $D_W$ value was obtained from CHEMDAT8 database in U.S. EPA (1994f). | 4.63E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | Geometric mean value obtained from Thompson, Burton, Quinn, and Ng (1972) for freshwater and marine fish. | 2.83E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-42

## CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | *RfD* value cited in U.S. EPA (1995c) for Chromium (III). | 1.5E+00 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 5.25E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 1E-01 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 7.4E+01 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-43

## CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 52 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 2,173.0 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.36E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.58E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 31 at pH=4.9;<br>19 at pH=6.8;<br>14 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 31 at pH=4.9;<br>19 at pH=6.8;<br>14 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCF* values were obtained from U.S. EPA (1995g) for all metals, except lead and mercury. | 3.0E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-43

## CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | *RfD* value cited in U.S. EPA (1997b) for Chromium (VI). | 5.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated based on *Inhalation URF* using inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 4.1E+01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.8E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | *Inhalation CSF* value cited in U.S. EPA (1997c) for Chromium (VI). | 4.1E+01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 1.1E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-44

# CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 228.28 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 527.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.03E-11 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.94E-03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 1.21E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 2.48E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 6.21E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.48E+05 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.97E+05 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.97E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.23E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.60E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.20E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.00E+01 |

## TABLE A-1a-44

## CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 6.03E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for chrysene of 0.001 (U.S. EPA 1993e) | 7.30E-03 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.30E-03 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-45

# CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 108.13 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 284.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.90E-04 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 2.30E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 8.93E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.93E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.30E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g) | 9.10E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.78E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.78E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.58E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.60E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 9.30E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.81E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-45

## CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.8E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-46

# CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 108.13 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 303.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 4.16E-04 at 25°C (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.77E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.62E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.88E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.41E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.05E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.34E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.34E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.00E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.10E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.60E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 9.80E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.02E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-46

## CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-47

# CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 108.13 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 308.6 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.70E-04 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 2.30E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.99E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.93E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.30E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g). | 8.70E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.61E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.61E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.46E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.60E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.90E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.75E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-47

## CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 5.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-48

# CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 120.19 |
| $T_m$ (K) | U.S. EPA (1995g) | 177 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 6.00E-03 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 5.60E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.29E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.50E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.83E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g) | 4.10E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.31E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.31E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.98E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.20E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.80E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.80E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.28E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-48

## CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 4.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-49

# CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | U.S. EPA (1992a) | 26.017 |
| $T_m$ (K) | -- | ND |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.82E-02 at 25ºC (solid) |
| *S* (mg/L) | -- | ND |
| *H* (atm·m$^3$/mol) | -- | ND |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 5.48E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 2.10E-05 |
| $K_{ow}$ (unitless) | -- | ND |
| $K_{oc}$ (mL/g) | -- | ND |
| $Kd_s$ (cm$^3$/g) | -- | ND |
| $Kd_{sw}$ (L/Kg) | -- | ND |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1998b) | 6.33E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | ND |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-02 |
| *Oral CSF* (mg/kg/day)$^{-1}$ | -- | ND |
| *RfC* (mg/m$^3$) | Calculated from *RfD* using an inhalation rate of 20 m$^3$/day and a human body weight of 70 kg. | 7.0E-02 |
| *Inhalation CSF* (mg/kg/day)$^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 2E-01 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 5.2E+00 |

## TABLE A-1a-49

## CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-50

# CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 320.05 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 380.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.14E-09 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.33E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.98E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.69E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.76E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.32E+06 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 4.58E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.58E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.44E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.60E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 7.80E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.70E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 5.25E+05 |

## TABLE A-1a-50

## CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 2.40E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 2.40E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 6.4E-03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-51

# CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 319.03 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 361.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 7.45E-09 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.92E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.24E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.70E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.78E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.80E+06 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 8.64E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.64E+06 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.48E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 7.60E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.60E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.80E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 5.53E+05 |

## TABLE A-1a-51

## CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 3.40E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 3.40E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.05E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-52

# CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 354.49 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 381.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 5.17E-10 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.41E-03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.37E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.48E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.48E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.17E+06 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 6.78E+05 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.78E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.08E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 5.70E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.30E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.00E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.40E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 4.30E+05 |

## TABLE A-1a-52

## CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 3.40E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 3.40E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 1.0E-03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-53

# CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 278.34 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 238.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 5.55E-08 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.08E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.43E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 4.38E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 7.86E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.25E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.57E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.57E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.18E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 7.20E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.20E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.10E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 5.58E+03 |

## TABLE A-1a-53

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 3.0E+01 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-54

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYL PHTHALATE (117-84-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 390.56 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 248.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 5.90E-09 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.00E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.68E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.32E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.20E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.14E+09 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.03E+08 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.03E+06 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.78E+07 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.20E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.10E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.90E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.10E+04 |

## TABLE A-1a-54

## CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYL PHTHALATE (117-84-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 3.88E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 2.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 1.99E+03 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-55

## CHEMICAL-SPECIFIC INPUTS FOR DIBENZ (A,H) ANTHRACENE (53-70-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 278.33 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 539.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.70E-14 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 6.70E-04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table. | 1.12E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 1.80E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 6.01E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 3.53E+06 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values was obtained from U.S. EPA (1996b). | 1.79E+06 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.79E+04 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.34E+05 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 2.10E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.10E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.90E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 1.28E+04 |

## TABLE A-1a-55

## CHEMICAL-SPECIFIC INPUTS FOR DIBENZ (A,H) ANTHRACENE (53-70-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 1.0 (U.S. EPA 1993e). | 7.30E+00 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.30E+00 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-56

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 236.36 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 279.2 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.0E-03 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.20E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.97E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.79E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.79E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 2.19E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.47E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.47E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.10E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.80E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.20E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.54E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-56

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1996d) | 5.70E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.40E+00 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 2.00E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1996d) | 2.40E-03 |
| *MCL* | National Primary Drinking Water Regulations. | 2E-04 |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-57

# CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 208.3 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 252.1 |
| *Vp* (atm) | *Vp* value cited in Montgomery and Weldom (1991). | 2.00E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 3.44E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.21E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.96E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.05E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994g). | 1.50E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 7.05E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.05E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.29E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.50E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.60E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.90E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.50E-02 |

## TABLE A-1a-57

## CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.65E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 8.40E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 8.4E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-58

# CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 147.01 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 256.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.79E-03 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.25E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.11E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.11E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.93E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.79E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 3.79E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.79E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.84E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 6.60E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.70E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | BCFs were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.45E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-58

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 9.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 2.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.4E+01 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-59

# CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 147.01 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 297.86 |
| *Vp* (atm) | *Vp* value cited in Howard (1989-1993). | 3.03E-03 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in Howard (1989-1993). | 6.88E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.11E+02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.14E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.85E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 3.39E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.03E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.03E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.02E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.10E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.00E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.84E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-59

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 8.90E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.12E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 7.1E+01 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-60

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 147.01 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 326.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.39E-03 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.30E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.80E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.14E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.85E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 2.58E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 6.16E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.16E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.62E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.60E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.31E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-60

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1996c) | 3.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 2.40E-02 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 8.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 2.40E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.5E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-61

# CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 253.13 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 405.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.89E-10 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.52E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.08E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.28E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.48E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 3.76E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.70E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.70E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.52E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.70E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.20E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.07E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-61

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | NA |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 4.50E-01 |
| *RfC* $(mg/m^3)$ | -- | NA |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 4.50E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-62

# CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 120.92 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 115.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 6.40E+00 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 3.0E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.58E+00 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.77E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 9.00E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.44E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 6.85E+0 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.85E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.14E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.20E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.80E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.40E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.58E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-62

## CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 2.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-63

# CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 98.97 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 175.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 3.0E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 5.16E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.75E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.42E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.05E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 6.20E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 5.30E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.30E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.98E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.90E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.50E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.40E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.20E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.36E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-63

## CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 9.1-E-02 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 5.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 9.1-E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.58E+03 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-64

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (ETHYLENE DICHLORIDE) (107-06-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 98.96 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 233.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.07E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 8.31E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.27E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.19E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.10E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.90E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.96E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.96E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.47E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.50E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.40E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.00E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L//kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 7.61E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-64

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (ETHYLENE DICHLORIDE) (107-06-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1996b) | 2.90E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 9.10E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 9.10E-02 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.0E+03 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-65

# CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 96.95 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 150.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 7.88E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.0E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.55E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.53E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.09E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.32E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 6.50E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.50E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.73E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.40E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.20E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.41E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-65

## CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 9.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 6.00E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.20E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.80E-01 |
| *MCL* | National Primary Drinking Water Regulations. | 7E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.03E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-66

# CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Howard (1989-1993) | 96.94 |
| $T_m$ (K) | Howard (1989-1993) | 192.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.30E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 4.94E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.51E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.36E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.13E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 9.60E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.98E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.98E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.85E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.40E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.40E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.20E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.20E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (unitless, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.89E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-66

## CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 7E-02 |
| *Aquatic* TRV (ug/l) | Suter (1996) | 5.72E+03 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-67

## CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 96.95 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 223.7 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 4.63E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 6.03E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.44E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 8.16E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 9.75E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 9.60E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 3.80E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.80E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.85E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.40E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.40E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.20E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.20E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.89E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-67

## CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 1E-01 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.4E+03 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-68

# CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 163.01 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 318.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 7.21E-06<br>at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 4.93E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.38E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.69E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.79E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 1.09E+03 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1-4 / 159.0<br>5 / 158.8<br>6 / 156.8<br>7 / 139.6<br>8 / 67.31<br>9 / 12.75<br>10 / 3.50<br>11 / 2.51<br>12 / 2.41<br>13-14 / 2.40 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.40E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.05E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.60E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.50E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.20E-01 |

## TABLE A-1a-68

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.19E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.6E+01 |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-69

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 112.99 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 172.7 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 6.66E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.68E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.81E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.21E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.71E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.78E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 4.70E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.70E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.53E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 9.80E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 9.30E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were obtained from U.S. EPA (1995g). | 3.02E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-69

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1996c) | 1.10E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c)) | 6.80E-02 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 4.00E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 6.80E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 5.25E+02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-70

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE (542-75-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 110.98 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 189.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 4.11E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.55E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.94E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.26E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.00E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 5.60E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.70E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.70E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.03E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.10E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.25E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-70

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE (542-75-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 1.8E-01 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 2.0E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.3E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 4.0E+01 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-71

## CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 380.93 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 449.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a) | 1.31E-09 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a) | 1.87E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.66E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 1.36E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 4.29E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 1.86E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.55E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.55E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.91E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 5.90E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.80E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.80E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.30E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 2.86E+04 |

## TABLE A-1a-71

## CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.60E+01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.6-E+01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 5.6E-02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-72

## CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 222.24 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 232.6 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.17E-06 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 8.80E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.48E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.56E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.35E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.73E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 8.20E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.20E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.15E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.00E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.80E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.20E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 2.45E+03 |

## TABLE A-1a-72

## CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 8.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.80E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 2.2E+02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-73

## CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 194.19 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 273.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.17E-06 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 4.19E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.01E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.96E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.13E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 4.30E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.09E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.09E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.32E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.60E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.70E-03 |

## TABLE A-1a-73

## CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.03E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 1.00E+01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E+01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.30E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-74

# CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Moses (1978) | 122.17 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 300.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a). | 1.66E-04<br>at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 6.25E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.27E-09 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.84E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.69E-06 |
| $K_{ow}$ (unitless) | Recommended $K_{ow}$ value cited in Karickhoff and Long (1995). | 2.29E+02 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1-5 / 126.0<br>6 / 125.99<br>7 / 125.9<br>8 / 125.02<br>9 / 116.87<br>10 / 71.06<br>11 / 15.77<br>12 / 3.43<br>13 / 2.05<br>14 / 1.91 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.26E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.44E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.60E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.30E-02 |

## TABLE A-1a-74

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.66E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.12E+01 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-75

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 244.28 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 410.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 3.30E-10 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 2.40E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.36E-10 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 2.38E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 5.60E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 6.46E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.65E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.65E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.74E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.70E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.50E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.50E-03 |

## TABLE A-1a-75

## CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.40E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.40E-02 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.40E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-76

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 168.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 363 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994f). | 4.0E-07 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994f). | 5.4E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 1.25E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 3.18E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 9.15E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994f). | 3.10E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.06E+01 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.06E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.55E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.10E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.20E-03 |

## TABLE A-1a-76

## CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 7.40E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-77

# CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 184.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 385.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.52E-07<br>at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 5.8E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.82E-09 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.73E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.06E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 3.30E+01 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1 / 0.80<br>2 / 0.79<br>3 / 0.72<br>4 / 0.38<br>5 / 0.08<br>6 / 0.02<br>7-14 / 0.01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0. | 1.0E-04<br>(at pH 7.0) |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.50E+04<br>(at pH 7.0) |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.80E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.80E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.50E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$<br>(L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 8.40E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-77

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 6.2E+00 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-78

# CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Howard (1989-1993) | 182.14 |
| $T_m$ (K) | Howard (1989-1993) | 344 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.29E-07 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.85E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 1.46E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 3.09E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 7.86E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 9.90E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.10E+01 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.10E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.82E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.90E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.70E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 5.92E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-78

## CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1995d) | 2.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | The *Oral CSF* value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 1997b). | 6.8E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 6.8E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.10E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-79

# CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Howard (1989-1993) | 182.15 |
| $T_m$ (K) | Howard (1989-1993) | 339 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 7.47E-07 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.05E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 1.30E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 3.11E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 7.76E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 7.70E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.19E+01 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.19E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.14E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.10E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.70E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.40E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 5.92E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-79

## CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | The *Oral CSF* value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 1997b). | 6.8E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.5E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 6.8E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.1E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-80

# CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 88.10 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 284.9 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 5.00E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 9.00E+05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.89E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.20E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.05E-05 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g) | 5.40E-01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.76E-01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.76E-03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.60E-02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.90E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.20E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.10E-05 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.69E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-80

## CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.1E-02 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 1.1E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-81

# CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 184.24 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 401.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 4.74E-08 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 6.80E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.28E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.95E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.24E-06 |
| $K_{ow}$ (unitless) | Montgomery and Welkom (1991) | 8.71E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.78E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.78E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.08E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.01E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-81

## CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 8.0E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 8.0E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.7E+00 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-82

# CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 274.38 |
| $T_m$ (K) | $T_m$ value cited in U.S. EPA (1995g). | 248 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 3.7E-07 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.6E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.12E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 4.50E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 5.21E-06 |
| $K_{ow}$ (unitless) | Recommended $K_{ow}$ value cited in Karickhoff and Long (1995). | 9.55E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.80E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.80E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.35E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.40E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 9.50E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.23E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-82

## CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 4.00E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.40E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-83

# CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 406.95 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 343.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a). | 1.72E-11 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 2.31E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.04E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.59E-03 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.76E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 3.02E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.04E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.04E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.53E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.10E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.70E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.90E+02 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.60E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-83

## CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.10E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 5.6E-02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-84

# CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 380.93 |
| $T_m$ (K) | U.S. EPA (1992a) | 473.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a) | 7.68E-10 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a) | 2.46E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.19E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 1.07E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 5.76E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 7.79E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.08E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.08E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.10E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 3.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.80E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.90E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.10E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 8.55E+03 |

## TABLE A-1a-84

## CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.10E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 2E-03 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 3.6E-02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-85

## CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (1-CHLORO-2,3-EPOXYPROPANE) (106-89-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 92.53 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 247.5 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 2.20E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 6.60E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.08E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.13E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.10E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.78E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.22E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.22E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.67E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 7.80E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.70E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.80E-04 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 9.13E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-85

## CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (1-CHLORO-2,3-EPOXYPROPANE) (106-89-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1995g) | 2.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 9.90E-03 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 1.00E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 4.20E-03 |
| *MCL* | National Primary Drinking Water Regulations. | TT[7] |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-86

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | *MW* value cited in U.S. EPA (1995g) | 114.14 |
| $T_m$ (K) | -- | NA |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 2.30E-02 at 25ºC |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.90E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.38E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.07E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 9.35E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 3.89E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.46E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.46E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.85E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 5.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.90E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 9.51E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-86

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 9.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.20E-01 |
| *Inhalation URF* $(\mu g/m^3)^{-1}$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-87

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 124.15 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 373.0 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 3.50E-04 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 4.90E+05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 8.87E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.63E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.84E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.12E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.55E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0. | 1.55E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.16E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.60E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.10E-04 |

## TABLE A-1a-87

## CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.42E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 2.93E+02 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 2.93E+02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-88

# CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 106.16 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 178.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.26E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.73E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.73E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.65E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.49E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.33E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.04E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.04E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.53E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 7.30E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.40E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.39E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-88

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 1.00E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 7E-01 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 4.53E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-89

# CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 187.88 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 282.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.00E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 4.20E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.47E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.17E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.19E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 5.62E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.28E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.28E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.46E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 2.40E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.90E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.60E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.26E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-89

## CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1996c) | 5.70E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 8.50E+01 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1995b) | 2.00E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Calculated from *Inhalation URF* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.70E-01 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-05 |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-90

## CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-ETHYLHEXYL) PHTHALATE (117-81-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 390.54 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 218.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 8.49E-09 at 25°C (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1998c). | 3.96E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 8.37E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.32E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.22E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.60E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.11E+05 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.11E+03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.32E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.30E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.10E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+02 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E+01 |

## TABLE A-1a-90

## CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-ETHYLHEXYL) PHTHALATE (117-81-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 3.60E+02 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.40E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 1.4E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 3.2E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-91

# CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 202.26 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 383.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.07E-08 at 25°C (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.32E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 9.33E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.75E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.18E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 1.21E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 4.91E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.91E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.68E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.80E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.50E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E+01 |

# TABLE A-1a-91

# CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 1.57E+04 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 4.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.4E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 4.0E+01 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-92

# CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 166.22 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 389.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 8.17E-07 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 1.90E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.30E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 3.63E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 7.88E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g) | 1.47E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 7.71E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.71E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.78E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.80E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.60E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 1.20E+03 |

## TABLE A-1a-92

## CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 4.00E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.40E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 4.0E+00 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-93

# CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 30.03 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 365.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1994c) | 5.10E+00 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 5.50E+05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.78E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 5.00E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 1.74E-05 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g) | 2.20E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.62E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.62E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.97E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.20E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.90E-05 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 1.07E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-93

## CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated from *Inhalation URF* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 4.50E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 4.50E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-94

# CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | U.S. EPA (1995g) | 46.03 |
| $T_m$ (K) | U.S. EPA (1995g) | 282.0 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 5.40E-02 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 1.00E+06 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.49E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.22E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.71E-05 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g) | 2.90E-01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.39E-01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.39E-03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.04E-02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.10E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.00E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.90E-05 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.30E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-94

## CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 2.00E+00 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-95

# CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 373.35 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 368.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 4.29E-07 at 25°C (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.73E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.87E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.12E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.69E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.04E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 9.53E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.53E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.15E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.80E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.70E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.80E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.80E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 5.52E+03 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-95

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 4.50E+00 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 4.50E+00 |
| *MCL* | National Primary Drinking Water Regulations. | 4E-04 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 3.8E-03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-96

# CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 389.32 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 430.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a). | 5.79E-09 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a) . | 2.68E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 8.29E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.32E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.23E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.62E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 7.18E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.18E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.38E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.90E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.10E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.00E+02 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E+01 |

## TABLE A-1a-96

## CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 5.88E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.30E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 9.1E+00 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 4.6E-05 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 9.1E+00 |
| *MCL* | National Primary Drinking Water Regulations. | 2E-04 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 3.8E-03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-97

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 260.76 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 252.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.33E-04 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.54E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.39E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.73E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.33E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.38E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 6.94E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.94E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.20E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.30E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.70E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.50E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 5.69E+03 |

## TABLE A-1a-97

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1995b) | 2.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 7.80E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 7.80E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 9.3E-01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-98

# CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 284.8 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 504.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 1.62E-08 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 8.62E-03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 5.35E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 1.41E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database U.S. EPA (1994d). | 7.84E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 3.18E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 8.00E+04 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.00E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.00E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 5.30E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.80E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.30E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.80E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 5.52E+04 |

## TABLE A-1a-98

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 8.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.6E+00 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.8E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.6E+00 |
| *MCL* | National Primary Drinking Water Regulations. | 1E-03 |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-99

# CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 272.77 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 264.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 9.63E-05 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.53E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.72E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.61E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.21E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 8.07E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.51E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.51E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.13E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 2.80E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.90E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.50E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 5.25E+02 |

## TABLE A-1a-99

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 7.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 7.00E-05 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 5E-02 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 7.0E-02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-100

# CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, Heckelman (1989) | 236.74 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 459.7 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 6.21E-04 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 4.08E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.60E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.77E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.88E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 9.66E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.82E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.82E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.36E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.00E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 6.29E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-100

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.40E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.40E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 9.8 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-101

# CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith and Heckleman (1989) | 406.92 |
| $T_m$ (K) | Budavari, O'Neil, Smith and Heckleman (1989) | 437.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 3.60E-15 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 3.0E-03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.88E-10 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 3.46E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 4.01E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 3.47E+07 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.08E+06 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.08E+04 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.10E+04 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.70E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+02 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.50E+03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 4.66E+03 |

## TABLE A-1a-101

## CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.00E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.10E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-102

# CHEMICAL-SPECIFIC INPUTS FOR INDENO (1,2,3-CD) PYRENE (193-39-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 276.34 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 435 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 1.88E-13 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.07E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 4.86E-09 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database U.S. EPA (1995d) | 1.90E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database U.S. EPA (1995d) | 5.66E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 8.22E+06 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.11E+06 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.11E+04 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.08E+05 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.10E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.20E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.00E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.50E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 1.31E+04 |

## TABLE A-1a-102

## CHEMICAL-SPECIFIC INPUTS FOR INDENO (1,2,3-CD) PYRENE (193-39-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Indeno(1,2,3-cd)pyrene of 0.1 (U.S. EPA 1993e). | 7.3E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.3E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-103

# CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 138.21 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 265.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a). | 5.38E-04 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.20E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.20E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.22E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.50E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.00E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.99E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.99E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.24E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.40E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.10E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.50E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.00E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.15E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-103

## CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 9.50E-04 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 9.50E-04 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.170E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-104

# CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 207.2 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 600.5 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 5.43E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 6.28E-06 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984), which states that several factors, such as experimental methods and soil type, could influence partitioning or $Kd_s$ values. Baes, Sharp, Sjoreen, and Shor (1984) compares values between various literature sources and provide this value, which is based on its best judgment. | 9.00E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 9.00E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | ND |
| $BAF_{fish}$ (day/kg FW) | Because lead is hydrophobic, *BAF* was used. $BAF_{fish}$ value was obtained from NC DEHNR (1997). | 8.0 |

## TABLE A-1a-104

## CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | Action level=1.5E-02; TT[6] |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 2.5E+00 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-105

## CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 200.59 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 234.23 |
| *Vp* (atm) | Budavari, O'Neil, Smith, and Heckelman (1989) | 2.63E-06 at 25°C |
| *S* (mg/L) | Budavari, O'Neil, Smith, and Heckelman (1989) | 5.62E-02 |
| *H* (atm·m$^3$/mol) | U.S. EPA (1997g) | 7.1E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate $D_a$ values. A density value of 13.546 g/cc for mercury was used. | 1.09E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate $D_w$ values. A density value of 13.546 g/cc for mercury was used. | 3.01E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | U.S. EPA (1997g) | 1.00E+03 |
| $Kd_{sw}$ (L/Kg) | U.S. EPA (1997g) | 1.00E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/g FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | Elemental mercury does not deposit onto soils and surface water. Therefore, there is no transfer of elemetal mercury into the fish tissue. | NA |

## TABLE A-1a-105

## CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | Calculated from *RfC* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 8.60E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | U.S. EPA (1997b) | 3.0E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 2E-03 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 7.7E-01 |

Note: NA = Not available, ND = No data available

# TABLE A-1a-106

# CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 67.09 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 237.3 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 8.90E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 2.50E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.39E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.15E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.33E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 3.47E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.74E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.74E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.81E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.80E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.40E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.50E-04 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.52E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-106

## CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 7.0E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-107

# CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 32.04 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 175.3 |
| *Vp* (atm) | *Vp* value cited in Montgomery and Welkom (1991) | 1.30E-01 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 2.90E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.44E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 4.58E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.64E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 1.95E-01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.96E-01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.96E-03 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.00E-02 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 3.80E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.40E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.30E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.90E-05 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.70E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-107

## CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.8E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-108

# CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 345.65 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 351.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.62E-09 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 8.84E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.33E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.30E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.59E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 3.36E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 8.00E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.00E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.00E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 6.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.10E+01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.40E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.20E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 3.16E+03 |

## TABLE A-1a-108

## CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 4E-02 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 3.0E-02 |

Note: NA = Not applicable, ND = No data available

## TABLE A-1a-109

## CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith and Heckelman (1989) | 94.95 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 179.44 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.16E+00 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.45E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.41E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.28E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.21E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.30E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 9.00E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.00E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.75E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.50E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.00E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.50E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.14E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-109

## CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.40E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 5.00E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.10E+02 |

.

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-110

# CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 50.49 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 176.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 5.68E+00 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 6.34E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.52E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.13E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.39E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 8.00E+00 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 6.00E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.00E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.50E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.80E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.30E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.10E-04 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.86E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-110

## CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | Calculated from *RfC* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 8.60E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995c) | 1.30E-02 |
| *RfC* ($mg/m^3$) | U.S. EPA (1997d) | 3.00E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 6.30E-03 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 5.5E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-111

# CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 72.10 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 187.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.20E-01 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 2.40E+05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.61E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.35E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.03E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.91E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.34E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.34E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.76E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.10E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.40E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.80E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.90E-04 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 9.61E-01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-111

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.00E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 1.00E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-112

# CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 100.16 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 188.4 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 2.50E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 2.00E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.25E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.59E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.36E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.55E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.20E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.20E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.00E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.30E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.60E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.60E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.50E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.73E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-112

## CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 8.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997a) | 8.0E-01 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1995b) | 8.0E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 8.0E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

## TABLE A-1a-113

## CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | U.S. EPA (1997g) | 216.0 |
| $T_m$ (°K) | -- | ND |
| *Vp* (atm) | -- | ND |
| *S* (mg/L) | -- | ND |
| *H* (atm·m$^3$/mol) | U.S. EPA (1997g) | 4.7E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1997g). | 5.28E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 6.11E-06 |
| $K_{ow}$ (unitless) | -- | ND |
| $K_{oc}$ (mL/g) | -- | ND |
| $Kd_s$ (mL/g) | U.S. EPA (1997g) | 7.00E+03 |
| $Kd_{sw}$ (L/Kg) | U.S. EPA (1997g) | 7.00E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | Default value cited in U.S. EPA (1997g) for a Trophic Level 4 fish. | 6.80E+06 |

## TABLE A-1a-113

## CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *Oral CSF* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.5E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not Applicable, ND = No data available

# TABLE A-1a-114

## CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 263.23 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 310.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1992a). | 1.30E-08 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 5.00E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.84E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.87E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.43E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g). | 7.20E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.40E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.40E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.80E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.40E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.50E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 8.50E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.90E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 8.74E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-114

## CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.54E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 8.8E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-115

# CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 173.86 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 220.4 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 2.20E+00 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.45E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.64E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 6.10E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.06E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 4.17E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.60E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.60E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.95E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.30E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.20E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.00E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-115

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 1.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.5E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 110 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-116

# CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 84.94 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 178.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 4.87E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.74E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.38E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.69E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.25E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.80E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.00E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.00E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.50E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.50E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.90E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.80E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L./kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.30E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-116

## CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 7.5E-03 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 3.0E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Calculated from the Inhalatioin URF using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.6E-03 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.93E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-117

## CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 128.16 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 353.3 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.17E-04 at 25°C (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.11E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.82E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 5.26E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d) | 8.92E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.36E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.19E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.19E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.92E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 7.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.30E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.15E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-117

## CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1995b) | 4.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.40E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 6.2E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-118

# CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 58.69 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 1,828 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.26E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.46E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 16 at pH=4.9;<br>65 at pH=6.8;<br>1,900 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 16 at pH=4.9;<br>65 at pH=6.8;<br>1,900 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995g) | 3.07E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-118

## CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.02E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 5.2E+01 |

Note: Note: NA = Not applicable, ND = No data available

# TABLE A-1a-119

# CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 138.12 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 342.1 |
| *Vp* (atm) | *Vp* value cited in Montgomery and Welcom (1991). | 1.07E-05 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in Montgomery and Welcom (1991). | 1.26E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.17E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.29E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.81E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 7.08E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.93E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.93E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.95E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.50E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-119

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 6.00E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 2.00E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-120

# CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 138.12 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 387.1 |
| *Vp* (atm) | -- | 1.07E-05 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in Montgomery and Welcom (1991) | 8.90E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. | 1.65E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.11E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.23E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 2.34E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.66E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.66E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.25E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.57E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.09E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.46E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.34E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 5.92E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-120

## CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 3.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.05E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-121

# CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 138.12 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 419.10 |
| *Vp* (atm) | -- | ND |
| *S* (mg/L) | *S* value cited in Montgomery and Welcom (1991) | 1.07E-05 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. | 1.65E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.31E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.75E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 2.46E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.72E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.72E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.29E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.33E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.09E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.46E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.04E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.00E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-121

## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 3.00E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.05E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-122

# CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 123.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 279.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 3.21E-04 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.92E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 2.06E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 5.43E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 9.43E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 6.80E+01 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.19E+02 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.19E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.90E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.80E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 4.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.90E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998) | 5.92E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-122

## CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 2.0E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.70E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-123

# CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 139.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 317.1 |
| *Vp* (atm) | *Vp* value cited in Howard (1989-1993). | 2.63E-04 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in Howard (1989-1993). | 2.50E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.46E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.44E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.19E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 6.17E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 3.53E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.53E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.65E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.12E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.17E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.48E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.31E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.35E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-123

## CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.5E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-124

# CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 139.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 386.1 |
| *Vp* (atm) | *Vp* value cited in Howard (1989-1993). | 1.32E-06 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in Howard (1989-1993). | 2.50E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 7.32E-09 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.30E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.61E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 8.13E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.37E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.37E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.28E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.13E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.17E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.48E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.13E-03 |

## TABLE A-1a-124

## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.67E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 6.20E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.17E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 8.28E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-125

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | *MW* value cited in U.S. EPA (1995g) | 158.20 |
| $T_m$ (K) | -- | NA |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 3.80E-04 at 25ºC |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 1.10E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.47E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 6.50E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 7.52E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 2.57E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.07E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.07E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.02E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.10E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.10E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.90E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.60E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.00E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-125

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 5.4E+00 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 5.4E+00 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-126

# CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 198.23 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 339.6 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 1.32E-04 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 3.50E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.99E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.12E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.35E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.06E+03 |
| $K_{oc}$ (mL/g) | Estimated value was obtained from U.S. EPA (1994c). | 3.27E+02, for pH range of 4.9 to 8.0 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.27E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.45E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.10E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.80E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.40E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.18E+02 |
| $BAF_{fish}$ (L/kg, FW) | -- | NA |

## TABLE A-1a-126

## CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 4.9E-03 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 4.9E-03 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 5.85E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-127

# CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 130.19 |
| $T_m$ (K) | -- | ND |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1998c). | 4.63E-03 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1998c). | 1.46E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.13E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.67E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.75E-06 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g). | 2.40E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.70E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.70E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.27E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.00E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.40E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.50E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.59E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-127

## CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 7.0E+00 |
| *RfC* $(mg/m^3)$ | | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 7.0E+00 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-128

# CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 250.34 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 358.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994f) | 3.10E-06 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994f) | 3.20E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.43E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.86E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.34E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 1.22E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 3.21E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.21E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.40E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 3.10E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.90E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.40E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.80E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 3.61E+04 |

## TABLE A-1a-128

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 8.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.8E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | US. EPA (1995f) | 5.0E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-129

# CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 295.36 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 417.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994f). U.S. EPA (1994c) cites value from Howard (1989-1993) | 3.10E-06 at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991). | 3.20E-02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 2.86E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 1.87E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 5.0E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994f). | 4.37E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.89E+03 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.89E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.42E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.90E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.50E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.80E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.40E+00 |

## TABLE A-1a-129

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 4.65E+02 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 3.03E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 2.6E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on Oral CSF assuming route-to-route extrapolation. | 2.6E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-130

# CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 266.35 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 463 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 7.11E-07<br>at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.34E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table. | 1.41E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 1.56E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d). | 8.01E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.20E+05 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1 / 19,949<br>2 / 19,918<br>3 / 19,604<br>4 / 16,942<br>5 / 7,333<br>6 / 1,417<br>7 / 504.9<br>8 / 408.7<br>9 / 399.1<br>10-14 / 398.1 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | pH / $K_{oc}$<br>1 / 199.5<br>2 / 199.2<br>3 / 196.0<br>4 / 169.4<br>5 / 73.33<br>6 / 14.17<br>7 / 5.05<br>8 / 4.09<br>9 / 3.99<br>10-14 / 3.98 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.78E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.90E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.70E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.80E+01 |

## TABLE A-1a-130

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.20E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 3.97E+02 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 3.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 1.2E-01 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on the Oral CSF assuming route-to-route extrapolation | 1.2E-01 |
| *MCL* | National Primary Drinking Water Regulations. | 1E-03 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 1.5E+01 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-131

# CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 178.22 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 371.1 |
| *Vp* (atm) | Geometric mean value calculated from values cited in Montgomery and Welkom (1991). | 1.35E-03 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in Lucius et al. (1992). | 1.28E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.88E-01 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.33E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.47E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 3.55E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.09E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.09E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.57E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.30E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.60E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.90E+00 |

## TABLE A-1a-131

## CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | Default *BAF* value recommended for use by U.S. EPA (1995g), when literature data were not available. | 3.30E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-132

# CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 94.11 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 314.0 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 5.74E-04<br>at 25°C (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 9.08E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.95E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.27E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.03E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 3.00E+01 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1-7 / 22.0<br>8 / 21.8<br>9 / 20.0<br>10 / 11.2<br>11 / 2.27<br>12 / 0.51<br>13 / 0.32<br>14 / 0.30 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.20E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.65E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.70E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.30E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.90E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.00E-03 |

## TABLE A-1a-132

## CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 7.81E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.1E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 2.56E-01 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-133

# CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 260.4 |
| $T_m$ (K) | -- | ND |
| *Vp* (atm) | *Vp* value cited in Montgomery and Welkom (1991). | 1.70E-06 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 3.80E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.16E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.05E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.88E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 6.46E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.33E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.33E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.97E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 2.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.50E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.50E-01 |

## TABLE A-1a-133

## CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.63E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 2.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-134

# CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 256.13 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 428.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 5.30E-07 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 1.50E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 9.05E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 4.71E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 5.45E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 3.24E+03 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 7.74E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.74E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.80E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.60E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.20E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.70E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.20E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.74E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-134

## CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 7.5E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.6E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-135

# CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 202.24 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 429.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 5.59E-09 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1992a). | 1.30E-01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.14E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.72E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.14E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.00E+05 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 6.80E+04 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.80E+02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.10E+03 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 4.70E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.50E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.30E+01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 1.19E+04 |

# TABLE A-1a-135

# CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-136

# CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 79.10 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 231.5 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 2.60E-02 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 3.00E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.86E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.10E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.08E-05 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 4.68E+00 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.72E+00 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.72E-02 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.54E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.90E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 6.40E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.70E-04 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.90E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-136

# CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.50E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-138

# CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 162.18 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 284.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.10E-04 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.50E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.19E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 4.06E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 7.16E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 4.57E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.68E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.68E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.26E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.50E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.00E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.60E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.19E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-138

## CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 1.80E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on Oral CSF assuming route-to-route extrapolation. | 1.80E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-139

# CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 78.96 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 490.1 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.03E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.20E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995f) | 1.29E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-139

## CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997c) | 5.0E-03 |
| Oral *CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.8E-02 |
| Inhalation *CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 5E-02 |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 5.0E+00 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-140

# CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 107.87 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 1,233.6 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 8.38E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 9.71E-06 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995f) | 2.04E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-140

## CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.80E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 1.2E-04 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-141

# CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 334.40 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 541.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 2.20E-13 at 25°C (solid) |
| *S* (mg/L) | Montgomery and Welkom (1991) | 1.50E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.90E-13 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.38E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.58E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 8.51E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 4.53E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.53E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.40E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.10E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.60E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.30E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.50E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.72E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-141

## CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70kg. | 1.1E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Note applicable, ND = No data available

# TABLE A-1a-142

# CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 104.14 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 242.5 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 8.21E-03 at 25°C (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 2.57E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.33E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.73E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.77E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 8.49E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 9.12E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.12E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.84E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.40E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.80E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.10E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 8.70E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 9.91E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-142

## CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 1.0E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 1E-01 |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-143

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8 -TETRACHLORODIBENZO (P) DIOXIN (1746-01-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | U.S. EPA (1994a) | 321.98 |
| $T_m$ (K) | U.S. EPA (1994a) | 578.1 |
| *Vp* (atm) | U.S. EPA (1994a) | 9.74E-13 at 25ºC (solid) |
| *S* (mg/L) | U.S. EPA (1994a) | 1.93E-05 |
| *H* (atm·m$^3$/mol) | U.S. EPA (1994a) | 1.60E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.27E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 6.81E-06 |
| $K_{ow}$ (unitless) | U.S. EPA (1994a) | 4.37E+06 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.69E+06 |
| $Kd_s$ (mL/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.69E+04 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.02E+05 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 3.80E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 6.30E+02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | -- | 9.16E+05 |

## TABLE A-1a-143

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8 -TETRACHLORODIBENZO (P) DIOXIN (1746-01-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD (mg/kg/day)* | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.5E+05 |
| RfC $(mg/m^3)$ | -- | ND |
| Inhalation CSF $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.5E+05 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 1.0 E-08 |

Note: NA = Not Applicable, ND = No Data Available

# TABLE A-1a-144

# CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 215.89 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 411.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 7.1E-06 at 25ºC (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.30E+00 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.18E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.11E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.75E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 4.36E+04 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 5.89E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.89E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 4.42E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.80E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.80E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.10E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.40E+00 |

## TABLE A-1a-144

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 4.30E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 5.0E+01 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-145

# CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 167.85 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 230.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g) | 1.60E-02 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g) | 1.10E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.44E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.15E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.30E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995) | 4.27E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.59E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.59E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.19E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.30E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.30E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.87E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-145

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 2.6E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 2.6E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-146

# CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 167.86 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 229.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 6.80E-03 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 3.07E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.72E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.16E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.26E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 4.40E+04 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 7.90E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.90E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.92E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 9.00E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.50E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g) | 4.33E+03 |

## TABLE A-1a-146

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 2.0E-01 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 2.0E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 4.2E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-147

# CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 165.85 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 251.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 2.42E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 2.32E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.73E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 7.20E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 8.20E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 3.51E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.65E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.65E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.99E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.50E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 9.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 4.70E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.06E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-147

## CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997e) | 5.2E-02 |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997d) | 4.0E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997e) | 2.0E-03 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.2E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-148

# CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | U.S. EPA (1995g ) | 231.89 |
| $T_m$ (K) | U.S. EPA (1995g) | 343.0 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 6.60E-06<br>at 25°C (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.00E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.53E-05 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 2.55E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 5.78E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.0E+04 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1 / 6,190<br>2 / 6,188<br>3 / 6,166<br>4 / 5,956<br>5 / 4,456<br>6 / 1,323<br>7 / 249.2<br>8 / 115.3<br>9 / 101.6<br>10 / 100.2<br>11-14 / 100.0 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a *pH* of 7.0. | 2.49 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.87E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.30E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.30E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.00E+00 |

## TABLE A-1a-148

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | -- | NA |
| $BAF_{fish}$ (L/kg FW) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g) | 1.63E+03 |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-149

# CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 204.38 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 576.6 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 5.48E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 6.34E-06 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | U.S. EPA (1998c) | 44 at pH=4.9;<br>71 at pH=6.8;<br>96 at pH=8.0 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 44 at pH=4.9;<br>71 at pH=6.8;<br>96 at pH=8.0 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995g) | 1.40E+03 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-149

## CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 8.0E-05 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.8E-04 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 2E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 4.00E+00 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-150

# CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 92.13 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 178.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 3.71E-02 at 25°C (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 5.58E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 6.13E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.72E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.23E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 4.65E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.40E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.40E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.05E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 4.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.20E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 7.70E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.60E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.27E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-150

## CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997b) | 4.0E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 1 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.3E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-151

# CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 107.15 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 258.4 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 3.94E-04 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.74E+04 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.43E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.14E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.12E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 2.19E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.57E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.57E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.18E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 3.80E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.50E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 2.20E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.14E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-151

## CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | NA |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 2.4E-01 |
| *RfC* $(mg/m^3)$ | -- | NA |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on Oral CSF assuming route-to-route extrapolation. | 2.4E-01 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-152

# CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 181.46 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 290.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 4.42E-04 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 3.07E+01 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 2.61E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.00E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.23E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 9.73E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.66E+03 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.66E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.24E+02 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.00E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.10E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.50E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.00E+00 |
| **Biotransfer Factors for Animals (Continued)** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 6.33E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-152

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 2.0E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 7E-02 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 1.11E+02 |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-153

# CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 133.42 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 242.7 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c) | 1.63E-01 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c) | 1.17E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.86E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.64E+02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.56E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c) | 2.64E+02 |
| $K_{oc}$ (mL/g) | Geometric mean value cited in U.S. EPA (1996b) | 1.35E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.35E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.01E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.10E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.70E-02 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.10E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.00E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.08E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-153

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 3.50E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | NA |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.23E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | 2E-01 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 5.28E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-154

# CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 133.42 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 238.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 3.31E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 4.40E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.00E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.51E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.0E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.25E+02 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 7.50E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.50E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 5.62E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 8.30E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 5.70E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.10E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 2.31E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-154

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 4.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 5.70E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.4E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 5.7E-02 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 9.40E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-155

# CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 131.40 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 188.3 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 9.48E-02 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 1.18E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.06E-02 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.65E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.94E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 2.71E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 9.40E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 9.40E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 7.05E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.60E-01 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 8.70E-02 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 2.10E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.10E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.16E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-155

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997a) | 6.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 1.1E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.1E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 6.0E-03 |
| *MCL* | National Primary Drinking Water Regulations. | 5E-03 |
| *Aquatic* TRV (ug/l) | U.S. EPA (1996c) | 3.5E+02 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-156

# CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 137.38 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 162.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.10E+00 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.10E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 1.37E-01 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 4.27E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.0E-05 |
| $K_{ow}$ (unitless) | $K_{ow}$ value cited in U.S. EPA (1995g). | 3.40E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.34E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.34E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.01E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 1.70E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.00E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.40E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.94E+01 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-156

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | U.S. EPA (1997c) | 7.0E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-157

# CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 197.46 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 340.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 2.15E-05<br>at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.53E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 5.64E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.91E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.03E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 7.41E+03 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1-3 / 2,380<br>4 / 2,377<br>5 / 2,353<br>6 / 2,139<br>7 / 1,127<br>8 / 223.7<br>9 / 56.14<br>10 / 37.94<br>11 / 36.10<br>12 / 35.92<br>13-14 / 35.90 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0. | 1.13E+01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.45E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 7.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.10E+01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 7.90E-01 |

# TABLE A-1a-157

# CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 5.14E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 1.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* ($mg/m^3$) | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 3.5E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-158

# CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 197.46 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 342.1 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 1.55E-05<br>at 25ºC (solid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.53E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 4.06E-06 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.62E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.08E-06 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 5.15E+03 |
| $K_{oc}$ (mL/g) | For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). | pH / $K_{oc}$<br>1 / 1,070<br>2 / 1,070<br>3 / 1,069<br>4 / 1,063<br>5 / 1,006<br>6 / 670.8<br>7 / 226.2<br>8 / 120.4<br>9 / 108.4<br>10 / 107.1<br>11-14 / 107.0 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0. | 2.26E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.70E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 5.00E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.40E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 9.20E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 5.00E-01 |

## TABLE A-1a-158

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.90E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | -- |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1995b) | 1.1E-02 |
| *RfC* $(mg/m^3)$ | -- | -- |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | -- |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | U.S. EPA (1995f) | 3.2E+00 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-159

# CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Montgomery and Welkom (1991) | 147.43 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 258.4 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 4.90E-03 at 25ºC (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 1.90E+03 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.80E-04 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 3.99E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 9.24E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.78E+02 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 8.05E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.10E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 6.04E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 9.50E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 6.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.70E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.80E-02 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 3.02E+01 |
| $BAF_{fish}$ (L/kg FW | -- | NA |

## TABLE A-1a-159

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 6.0E-03 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 7.0E+00 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 2.1E-02 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | Value based on *Oral CSF* assuming route-to-route extrapolation. | 7.0E+00 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-160

# CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neill, Smith, and Heckelman (1989) | 213.11 |
| $T_m$ (K) | Budavari, O'Neill, Smith, and Heckelman (1989) | 395.6 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1995g). | 1.30E-07 at 25°C (solid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1995g). | 3.20E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 8.66E-08 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 2.84E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d). | 6.08E-06 |
| $K_{ow}$ (unitless) | Arithmetic mean value cited in Karickhoff and Long (1995). | 1.51E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.18E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.18E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.85E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 6.57E-04 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.75E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.19E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.51E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 4.64E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-160

## CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-02 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E-01 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA= Not applicable, ND= No data available

# TABLE A-1a-161

# CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 227.13 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 353.2 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 2.63E-07 |
| *S* (mg/L) | *S* value cited in U.S. EPA (1998c). | 1.30E+02 |
| *H* (atm·m$^3$/mol) | *H* value cited in U.S. EPA (1998c). | 4.59E-07 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 2.62E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 5.85E-06 |
| $K_{ow}$ (unitless) | Recommended $K_{ow}$ value cited in Karickhoff and Long (1995). | 3.98E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 2.51E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.51E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.88E+00 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | $K_p^{\ w}$ value was obtained from U.S. EPA (1992b). | 1.31E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 1.75E+00 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 4.19E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.98E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 9.68E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-161

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 5.0E-04 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 3.0E-02 |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.8E-03 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997b) | 3.0E-02 |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-162

# CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 62.50 |
| $T_m$ (K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 119.3 |
| *Vp* (atm) | Geometric mean value cited in U.S. EPA (1994c). | 3.68E+00 at 25ºC (liquid) |
| *S* (mg/L) | Geometric mean value cited in U.S. EPA (1994c). | 7.30E+02 |
| *H* (atm·m$^3$/mol) | *H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table. | 3.15E-01 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.58E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 1.19E-05 |
| $K_{ow}$ (unitless) | Geometric mean value cited in U.S. EPA (1994c). | 1.40E+01 |
| $K_{oc}$ (mL/g) | $K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table. | 1.11E+01 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.11E-01 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 8.33E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 9.20E-03 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 2.10E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 5.10E-01 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 3.20E-03 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg, FW tissue) | *BAFs* were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995g). *FCM*s were obtained from U.S. EPA (1995g) | 4.37E+00 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-162

## CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | -- | ND |
| *Oral CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 1.9E+00 |
| *RfC* $(mg/m^3)$ | -- | ND |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | U.S. EPA (1997c) | 3.0E-01 |
| *MCL* | National Primary Drinking Water Regulations. | 2E-03 |
| *Aquatic* TRV (ug/l) | -- | ND |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-163

# CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 106.16 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 225.7 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 1.06E-02 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1998c). | 1.86E+02 |
| *H* (atm·m$^3$/mol) | *H* value cited in U.S. EPA (1998c). | 6.05E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.69E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.49E-06 |
| $K_{ow}$ (unitless) | Recommended $K_{ow}$ value cited in Karickhoff and Long (1995). | 1.59E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 1.96E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.96E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.47E-01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 7.60E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.50E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.60E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-163

## CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E+00 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 2.7E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-164

# CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 106.16 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 248.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 1.06E-02 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1998c). | 1.86E+02 |
| *H* (atm·m$^3$/mol) | *H* value cited in U.S. EPA (1998c). | 6.05E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.69E-02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.44E-06 |
| $K_{ow}$ (unitless) | Recommended $K_{ow}$ value cited in Karickhoff and Long (1995). | 1.35E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 2.41E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.41E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 1.80E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 7.60E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.50E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.41E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-164

## CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E+00 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 2.7E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-165

# CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 106.16 |
| $T_m$ (K) | Montgomery and Welkom (1991) | 286.1 |
| *Vp* (atm) | *Vp* value cited in U.S. EPA (1998c). | 1.06E-02 at 25°C (liquid) |
| *S* (mg/L) | *S* value cited in U.S. EPA (1998c). | 1.86E+02 |
| *H* (atm·m$^3$/mol) | *H* value cited in U.S. EPA (1998c). | 6.05E-03 |
| $D_a$ (cm$^2$/s) | $D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 7.61E+02 |
| $D_w$ (cm$^2$/s) | $D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d). | 8.50E-06 |
| $K_{ow}$ (unitless) | Recommended $K_{ow}$ value cited in Karickhoff and Long (1995). | 1.48E+03 |
| $K_{oc}$ (mL/g) | Geometric mean of measured values obtained from U.S. EPA (1996b). | 3.11E+02 |
| $Kd_s$ (cm$^3$/g) | $Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$, because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 3.11E+00 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table. | 2.33E+01 |
| **Dermal Exposure Factors** | | |
| $K_p^w$ (cm/hr) | $K_p^w$ value was obtained from U.S. EPA (1992b). | 7.60E-02 |
| *t* | *t* value was obtained from U.S. EPA (1992b). | 3.90E-01 |
| *t** | t* value was obtained from U.S. EPA (1992b). | 1.30E+00 |
| *B* | *B* value was obtained from U.S. EPA (1992b). | 1.50E-01 |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | *BCFs* were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995g). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980) | 1.51E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

# TABLE A-1a-165

## CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 2.0E+00 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 7.0E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Suter (1996) | 2.7E+03 |

Note: NA = Not applicable, ND = No data available

# TABLE A-1a-166

# CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Chemical/Physical Properties** | | |
| *MW* (g/mole) | Budavari, O'Neil, Smith, and Heckelman (1989) | 65.38 |
| $T_m$ (°K) | Budavari, O'Neil, Smith, and Heckelman (1989) | 692.6 |
| *Vp* (atm) | All metals, except mercury, are assumed to be nonvolatile at ambient temperatures. | 0.0 |
| *S* (mg/L) | All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989) | 0.0 |
| *H* (atm·m$^3$/mol) | *H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury. | 0.0 |
| $D_a$ (cm$^2$/s) | $D_a$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.17E-01 |
| $D_w$ (cm$^2$/s) | $D_w$ value was calculated using the equation cited in U.S. EPA (1996a). | 1.36E-05 |
| $K_{ow}$ (unitless) | -- | NA |
| $K_{oc}$ (mL/g) | -- | NA |
| $Kd_s$ (mL/g) | $Kd_s$ value was obtained from U.S. EPA (1996), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. | 6.2E+01 at pH=6.8 |
| $Kd_{sw}$ (L/Kg) | $Kd_{sw}$ value is assumed to be the same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). | 6.2E+01 at pH=6.8 |
| **Dermal Exposure Factors** | | |
| $K_p^{\ w}$ (cm/hr) | -- | ND |
| *t* | -- | ND |
| *t** | -- | ND |
| *B* | -- | ND |
| **Biotransfer Factors for Animals** | | |
| $BCF_{fish}$ (L/kg FW tissue) | U.S. EPA (1995g) | 6.54E+02 |
| $BAF_{fish}$ (L/kg FW) | -- | NA |

## TABLE A-1a-166

## CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

| Parameter | Reference and Explanation | Value |
|---|---|---|
| **Health Benchmarks** | | |
| *RfD* (mg/kg/day) | U.S. EPA (1997b) | 3.0E-01 |
| *Oral CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *RfC* $(mg/m^3)$ | Calculated from *RfD* using an inhalation rate of 20 $m^3$/day and a human body weight of 70 kg. | 1.1E+00 |
| *Inhalation CSF* $(mg/kg/day)^{-1}$ | -- | ND |
| *MCL* | National Primary Drinking Water Regulations. | ND |
| *Aquatic* TRV (ug/l) | Ambient Water Quality Criteria, U.S. EPA, Office of Water. | 1.20E+02 |

Note: NA = Not applicable, ND = No data available