APPENDIX A

CHEMICAL-SPECIFIC DATA

DELISTING TECHNICAL SUPPORT DOCUMENT

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

APPENDIX A-1

CHEMICAL INFORMATION ON DRAS WASTE CONSTITUENTS

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Attachment

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 (mg Chemical/kg FW tissue)/(mg Chemical/L total water column) 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 (mL water/g bottom sediment OR cm^3 water/g bottom sediment)
K_{ow}	=	Octanol/water partitioning coefficient (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)
τ	=	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 1×10^{-06} to 1×10^{-05} cm^2/s; therefore, U.S. EPA (1995a) recommended a default value of 8×10^{-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:

$$f_{fd} = \frac{1}{1 + \frac{(DOC)\ (K_{ow})}{10} + (POC)\ (K_{ow})}$$ 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 = 2×10^{-6} kg/L
POC = 7.5×10^{-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:

$$Inhal.\ URF = \frac{Oral\ CSF \cdot 20\ m^3/d}{70\ kg \times 1000\ \mu g/mg}$$ 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:

$$Inhal.\ CSF = \frac{Inhal.\ URF \cdot 70\ kg}{20\ m^3/d} \times 1000\ \mu g/mg$$ 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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APPENDIX A-1

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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 25°C (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 (^{o}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 (^{o}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; 29 at pH=6.8; 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; 29 at pH=6.8; 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; 41 at pH=6.8; 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; 41 at pH=6.8; 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 25°C (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 (^{o}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 (^{o}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 (^{o}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 at 25°C (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} 1-4 / 398.0 5 / 397.9 6 / 396.9 7 / 387.3 8 / 311.8 9 / 108.7 10 / 19.43 11 / 7.39 12 / 6.14 13 / 6.01 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 (^{o}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 (^{o}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; 19 at pH=6.8; 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; 19 at pH=6.8; 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 25°C (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 25°C (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 25°C (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 25°C (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 25°C (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 at 25°C (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} 1-4 / 159.0 5 / 158.8 6 / 156.8 7 / 139.6 8 / 67.31 9 / 12.75 10 / 3.50 11 / 2.51 12 / 2.41 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 25°C (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 at 25°C (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} 1-5 126.0 6 125.99 7 125.9 8 125.02 9 116.87 10 71.06 11 15.77 12 3.43 13 2.05 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 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} 1 0.80 2 0.79 3 0.72 4 0.38 5 0.08 6 0.02 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 (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 (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} (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 25°C (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 25°C (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 25ºC (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 25ºC (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 Caroll (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 25ºC (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 25ºC (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 25ºC (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 (^{o}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 (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	234.23
Vp (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	2.63E-06 at 25^{o}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 (^oK)	--	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 25°C (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 25°C (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; 65 at pH=6.8; 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; 65 at pH=6.8; 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 25°C (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 25°C (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 25°C (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 at 25°C (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} 1 19,949 2 19,918 3 19,604 4 16,942 5 7,333 6 1,417 7 504.9 8 408.7 9 399.1 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} 1 199.5 2 199.2 3 196.0 4 169.4 5 73.33 6 14.17 7 5.05 8 4.09 9 3.99 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 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} 1-7 / 22.0 8 / 21.8 9 / 20.0 10 / 11.2 11 / 2.27 12 / 0.51 13 / 0.32 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 Caroll (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 (^{o}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 (^{o}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 25°C (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 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} 1 6,190 2 6,188 3 6,166 4 5,956 5 4,456 6 1,323 7 249.2 8 115.3 9 101.6 10 100.2 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 (^{o}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; 71 at pH=6.8; 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; 71 at pH=6.8; 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 25°C (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 25°C (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 25°C (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 25°C (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 at 25°C (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} 1-3 / 2,380 4 / 2,377 5 / 2,353 6 / 2,139 7 / 1,127 8 / 223.7 9 / 56.14 10 / 37.94 11 / 36.10 12 / 35.92 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 at 25°C (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} 1 / 1,070 2 / 1,070 3 / 1,069 4 / 1,063 5 / 1,006 6 / 670.8 7 / 226.2 8 / 120.4 9 / 108.4 10 / 107.1 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 25°C (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

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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