APPENDIX A

CHEMICAL-SPECIFIC DATA

DELISTING TECHNICAL SUPPORT DOCUMENT

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U.S. Environmental Protection Agency
RCRA Delisting Team

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 the U.S. Environmental Protection Agency (U.S. EPA). 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 atmospheric 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 concentration 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 have become more available and are often found to have been measured with higher quality or estimated with better validation. EPA completed a comprehensive review of available Henry's Law constants in 2020 with many new values identified.

Organics and Elemental Mercury For organics and elemental mercury, Henry's Law Constant values were selected based on the approach outlined in "Finding and Estimating Chemical Property Data for Environmental Assessment" (Boethling et al. 2014) which was written by U.S. EPA and Syracuse Research Corporation scientists. This paper provides practical guidance on finding measured values and using estimation methods and states that "the cardinal rule in estimating chemical properties should be, if reliable measured values are available, ''don't do it.'' The following summarizes the approach used in selecting Henry's Law Constants for organics:

1. If a reliable measured (experimental) value was available, this value was prioritized over a theoretical estimated value. The following sources were used to find measured Henry's Law Constants.
    a. Sander, R. 2015, Compilation of Henry's law constants (version 4.0) for water as Solvent, Atmospheric Chemistry and Physics, 15, 4399-4981, Copernicus Publications, Gottingen, Germany.
        i. This resource contains a compilation of 17,350 Henry's Law Constants values for 4,632 chemicals. Some chemicals have several measured values. For example, there are 24 measured Henry's Law Constant values for acetone.
        ii. It includes an evaluation of quality similar to EPA's approach in the Boethling paper.
    b. EPI Suite™ (U.S. EPA 2020e).
        i. EPI Suite is a program developed by the U.S. EPA Office of Pollution Prevention and Toxics and Syracuse Research Corporation.
        ii. It is a screening level tool for calculating many chemical properties, one of which is the Henry's Law Constant.
        iii. It contains experimental values for Henry's Law Constants in addition to calculated values.

    References for chosen measured values tended to be the most recent ones listed in Sander (2015) and were reviewed for reliability. In addition, the mean and standard deviation (SD) of the measured values in Sander (2015) were calculated where multiple values of good quality were referenced. Of the experimentally measured H values in DRAS4, 65 percent were with one SD of the mean and 22 percent only had one measured value (therefore, no SD or mean could be calculated). The remaining 13 percent were within 2 or more SDs of the mean. In summary, most of the measured values were similar to other reported values and the few chosen values that were much different were measured based on reliable experimental techniques.

2. If a measured value was not available for a chemical, then a calculated theoretical value was used for the Henry's Law constant. The value chosen was the most conservative H value calculated. Higher H (atm-m^3/mol) results in higher risk and lower delisting levels in DRAS; therefore, the higher H value (atm-m^3/mol) was selected as the most conservative value. Calculated values

reviewed were those in EPI Suite (Bond Estimated and Group Estimated), the Vp/S equation, and calculated values in Sander (2015). H values calculated using the Vp/S equation are from the following theoretical equation (Lyman, Reehl, and Rosenblast 1982), using

$$H = \frac{Vp \bullet MW}{S} \qquad \text{Equation A-1-1}$$

recommended *MW, S,* and *Vp* values:

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)

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

Methyl Mercury The *H* value for methyl mercury was 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 water body.

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):

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}}$$ Equation A-1-2a

$$D_{w,i} = \frac{22\times10^{-5}}{(MW_i)^{2/3}}$$ Equation A-1-2b

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

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

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

Octanol/Water Partitioning Coefficient (K_{ow})

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

Organics EPI Suite™ version 4.11 (U.S. EPA 2020e) was used to update DRAS K_{ow} values. The EPI Suite program accesses the PHYSPROP database which is a database of physical properties of chemicals maintained by the Syracuse Research Center. KOWWIN is a program within EPI Suite that provides experimental references as well as a chemical structure-based model estimate of K_{ow}. Both PHYSPROP and KOWWIN were utilized for the selection of K_{ow} values. As with H value selection, if a reliable measured (experimental) value was available, this value was prioritized over a theoretical estimated value.

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 An experimental K_{ow} value for total mercury was obtained through KOWWIN. KOWWIN's estimated K_{ow} for methyl mercury was selected for DRAS.

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 over predict 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 DRAS 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 was used:

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

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

- Veith, G.D., K.J. Macek, S.R. Petrocelli, and J. Caroll. 1980. "An Evaluation of Using Partition Coefficients and Water Solubility to Estimate Bioconcentration Factors for Organic Chemicals in Fish." *Journal of Fish. Res. Board Can.* Prepublication Copy.

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

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

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

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

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

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

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

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

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

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

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

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

and, for the littoral ecosystem by the following:

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

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

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

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

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

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

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

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

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

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

where

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

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

DOC = 2×10^{-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

DRAS incorporates human health benchmarks as reference doses and reference concentrations for noncarcinogens, and as cancer slope factors for carcinogens. Reference dose (*RfD*) is defined as a daily intake rate via ingestion 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 via inhalation over a specific exposure duration (U.S. EPA 1989). EPA defines cancer slope factors as " used to estimate the risk of cancer associated with exposure to a carcinogenic or potentially carcinogenic substance. A slope factor is an upper bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime exposure to an agent by ingestion [or inhalation]".

Updated Toxicity Data

U.S. EPA reviewed all existing toxicity reference data in DRAS for outdated or errant values. To do so, U.S. EPA downloaded the May 2020 version of the Regional Screening Levels (RSLs) Generic Summary Tables (U.S. EPA 2020a) and compared toxicity reference values to those in DRAS. The RSLs replaced the Region 9 Preliminary Remediation Goals (PRGs) that were consulted for a previous version of DRAS (DRAS3). If an updated value was available, the value was changed in DRAS. In addition, the sources of the values were checked to verify the toxicity values. Some chemicals in DRAS were not listed in the RSL tables. In these instances, EPA followed the same hierarchy approach, described below, for selecting toxicity values as was done in the RSL tables.

Some of the updates were straightforward such as an unambiguous revision to the Integrated Risk Information System (IRIS – EPA's highest standard source for toxicity data). Other discrepancies required the review of Agency toxicologists in determining the appropriate default data for use in DRAS. In consideration of the exposure scenarios evaluated in the delisting program, U.S. EPA selected toxicity data in accordance with the hierarchy described in the December 2003 Memorandum from Michael B. Cook (U.S. EPA 2003), as did U.S. EPA in developing the RSL Tables. The types of pathway evaluations are very similar to those applied for Superfund-site evaluations. The hierarchy is as follows:

> IRIS is the first tier of the recommended hierarchy as the generally preferred source of human health toxicity values. IRIS generally contains reference doses (RfDs), reference concentrations (RfCs), cancer slope factors, drinking water unit risk values, and inhalation unit risk values that have gone through a peer review and EPA consensus review process. IRIS normally represents the official Agency scientific position regarding the toxicity of the chemicals based on the data available at the time of the review.
>
> The second tier is U.S. EPA's Provisional Peer Reviewed Toxicity Values (PPRTVs). PPRTVs are derived by U.S. EPA's Superfund Health Risk Technical Support Center (STSC). PPRTVs are derived after a review of the relevant scientific literature using the methods, sources of data and guidance for value derivation used by the U.S. EPA IRIS Program. All PPRTVs received internal review by U.S. EPA scientists and external peer review by independent scientific experts. PPRTVs are removed when an IRIS profile is released, even if the IRIS profile indicates a toxicity value could not be derived. PPRTVs retain subchronic values if IRIS releases a profile without subchronic values.

The third tier includes other sources of information. Priority should be given to sources that provide toxicity information based on similar methods and procedures as those used for Tier I and Tier II, contain values which are peer reviewed, are available to the public, and are transparent about the methods and processes used to develop the values. Consultation with the STSC or headquarters program office is recommended regarding the use of the Tier 3 values for Superfund response decisions when the contaminant appears to be a risk driver for the site. In general, draft toxicity assessments are not appropriate for use until they have been through peer review, the peer review comments have been addressed in a revised draft, and the revised draft is publicly available. These third-tier sources include:

- U.S. EPA's Office of Pesticide Programs (OPP) Human Health Benchmarks for Pesticides (HHBPs);
- The Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs);
- The California Environmental Protection Agency (CalEPA) Office of Environmental Health Hazard Assessment (OEHHA) toxicity values for the State of California; and
- The U.S. EPA Superfund program's 1997 Health Effects Assessment Summary Table (HEAST).

Explanation of Calculated Toxicity Benchmark Values – Route-to-Route Extrapolation

To calculate missing benchmarks, available benchmarks can be employed using a methodology referred to as *route-to-route extrapolation*. Route-to-route extrapolation is when a toxicity factor for one route of exposure (i.e. ingestion) is converted into a toxicity factor for another route of exposure (i.e. inhalation). A previous version of DRAS (DRAS3) included route-to-route extrapolations from the R9 2004 PRGs based on criteria set forth in "Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry" (U.S. EPA 1994g) and these extrapolations were carried over to the updated version of DRAS (DRAS4). For DRAS4, a subset of the toxicity data was re-evaluated for the use of route-to-route extrapolations (the RSL tables did not include route-to-route extrapolations). Specifically, EPA believed that the most appropriate way to evaluate a large group of chemicals for route-to-route extrapolations was by applying the following criteria from the 1994 report:

Oral data should not be used for route-to-route extrapolation in the following instances:
(1) when groups of chemicals are expected to have different toxicity by the two routes; for example, metals, irritants, and sensitizers;
(6) when short-term inhalation studies, dermal irritation, in vitro-studies, or characteristics of the chemical indicate potential for portal-of-entry effects at the respiratory tract, but studies themselves are not adequate for an RfC development.

The following databases were used for the evaluation:

(a) EPA's database for chemicals determined to be extremely hazardous substances after release to ambient air. These include chemicals assigned an EPA Level of Concern (LOC) as found in the document: "Technical Guidance for Hazards Analysis: Emergency Planning for Extremely Hazardous Substances" (U.S. EPA 1987);

(b) Emergency Planning Response Guideline (ERPG) values for protection of the general public from the acute toxic and/or debilitating effects of chemicals in ambient air. ERPGs are developed by the American Industrial Hygiene Association (http://www.orau.gov/emi/scapa/erpgdefinitions.htm) (AIHA 2005);

(c) U.S. DOE Temporary Emergency Exposure Limit (TEEL) values for protection of Federal workers and contractors at DOE facilities from the acute toxic and/or debilitating effects of chemicals in ambient air. TEELs are developed by methodologies similar to the ERPGs but include more chemicals (http://www.orau.gov/emi/scapa/teels.htm) (U.S. DOE 2005) ; and

(d) NIOSH Recommended Exposure Limit (REL) values for work place exposure. This encompasses chemicals that have been assigned a specific time-concentration exposure limit in ambient air because they are documented to be respiratory irritants (even for a healthy worker) in ambient air in the absence of exposure protection. (www.cdc.gov/niosh/92-100.html) (U.S. DHHS 1992).

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (a) include:

Acrylamide; Aldrin; Benzyl Chloride; o-Cresol; Endosulfan; Endrin; Disulfoton; Furan; N-Nitrosodimethylamine; Parathion; Pentachlorophenol; Phenylmercuric acetate; Phorate;

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (b) include:

Allyl chloride; Benzyl Chloride; Carbon tetrachloride; Methanol; Phenol; Trichloroethane (-1,1,1 and -1,1,2); Hexachlorobutadiene

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (c) include:

Acrylamide; allyl chloride; aniline; benzo[a]pyrene; 2,4-dinitrophenol; dibenzo[a,h]anthracene; strychnine; hexachloroethane; hexachlorophene; chloromethane; tribromomethane; methanol; heptachlor; 1,2-dichloropropane; 1,1,2-trichloroethane; 1,1,2,2-tetrachloroethane; 1,1,1,2-tetrachloroethane; pentachloronitrobenzene; diethylphthalate; dibutylphthalate; pentachlorophenol; 2-chloronaphthalene; 3,3Æ-dichlorobenzidene; o-cresol; p-cresol; m-cresol; o-toluidene; 2-chlorophenol; 1,2,4,5-tetrachlorobenzene; 2,4,5-trichlorophenol; 1,3,5-trinitrobenzene; 1,3-dinitrobenzene; p-chloroaniline; pyridine; hexachlorobenzene; hexachlorobutadiene; 3,3-dimethoxybenzidine; 2,4-dichlorophenol; pentachlorobenzene; DDE;

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (d) include:

Acetone - nose and throat irritant
Acetonitrile - nose and throat irritant
Bromoform - respiratory irritant
Dichlorobenzenes (all isomers) - upper respiratory irritants
Dichloroethylenes (all isomers) - mucous membrane irritants; narcosis;
Dimethylphthalate - upper respiratory irritant

Ethyl acetate - respiratory and eye irritant
Methyl acetate - upper respiratory irritant
Pentachlorophenol - upper respiratory irritant
Phenylenediamine - bronchial irritant and asthma inducer
Strychnine - convulsions
Trichloropropane - mucous membrane irritant; narcosis;

Consequently, for the above four lists of chemical constituents, we recommended against using route-to-route extrapolation from oral route data to derive inhalation toxicity factors.

For the remainder of the chemicals in the R9 2004 PRGs where extrapolation was used, the use of the route-to-route extrapolation in DRAS could be adopted on the basis that direct exposure effects of the remaining chemicals on the lung or respiratory system (of humans or animals) could not be identified. However, there could still be some significant uncertainties in the reliability of inhalation toxicity factors derived in this way. The primary uncertainty would probably be due to the rate of metabolism of a given chemical in the liver or lung and how that factor affects the ultimate level of absorption and transport to target organs. In the event that one of these route-to-route values becomes the basis for potentially denying a delisting petition, U.S. EPA Region 5 recommends that the reference value be further investigated to reduce this uncertainty. In order to carry on the evaluation further, published literature studies on the metabolism or pharmacology of the individual chemicals would need to be located and reviewed.

The discussion above covers the concept of using route-to-route extrapolation from oral route data to derive inhalation toxicity factors. In the R9 2004 PRGs, there were also some instances where DRAS lists oral toxicity factors that were apparently derived from IRIS verified inhalation toxicity factors. The use of this extrapolation procedure would also be subject to uncertainty. For the purposes of making an expedited screening level evaluation, we propose the following caveat: the route-to-route extrapolation from inhalation to oral should only be used when there is well documented evidence that exposure via the inhalation route results in adverse effects at organs or organ systems that are distant from the lung and respiratory tract (e.g., liver, kidney, thyroid, sex organs). The evaluation based on applying the above caveat is shown below:

RfD_O for Acetonitrile: IRIS reports health effects distant from the lung, therefore the route-to-route extrapolation is satisfactory.

RfD_O for Benzyl chloride: R9 lists an RfC referenced to National Center for Environmental Assessment (NCEA). We recommend not using the route-to-route extrapolation until we are able to verify the health effects reported in this reference.

RfD_O for Chlorodifluoromethane: IRIS reports health effects distant from the lung, therefore the route-to-route extrapolation is satisfactory.

RfD_O for Chloromethane: Because IRIS states that exposure to chloromethane can essentially occur only through the vapor phase, derivation of an oral toxicity factor is not necessary.

RfD_O for 3-Chloropropene (Allyl chloride): IRIS reports peripheral neurological effects in humans and liver and kidney degenerative effects in lab animals; under the assumption that oral exposure to Allyl Chloride could occur, the route-to-route extrapolation is satisfactory;

RfD_O for 1,2-Dichloropropane: IRIS reports that the observed adverse effects were seen only in the nasal tissue and respiratory epithelium; therefore, route-to-route extrapolation should not be used;

RfD_O for 2-Nitropropane: IRIS reports development of focal hepatocellular nodules and focal liver necrosis in lab animals with no significant effects on the respiratory tract; under the assumption that oral exposure could occur to Nitropropane, the route-to-route extrapolation is satisfactory.

Provisional Toxicity Data, Multiple CAS ID Numbers, Multiple Valence States, and Data Based on a Mixture of Compounds

Approximately 26 potential waste constituents have provisional toxicity data, multiple CAS identification numbers, valence states, or toxicity data based on a mixture of compounds. We individually evaluated these using the following acronyms and conversion algorithms:

CSF_O – Oral Cancer Slope Factor
CSF_I – Inhalation Cancer Slope Factor
IUR – Inhalation Unit Risk (cancer)

RfD_O – Oral Reference Dose
RfD_I – Inhalation Reference Dose
RfC – Inhalation Reference Concentration

CalEPA – California EPA

Conversion of RfC to RfD_I:

$$RfD_I\ (mg/kg\text{-}day) = RfC\ (mg/m^3) \times (20\ m^3/day) \times (1/72\ kg) \qquad \text{Equation A1-7}$$

Conversion of IUR to CSF_I:

$$CSF_I = IUR(ug/m^3)^{-1} \times (1\ day/20\ m^3) \times (72\ kg) \times (1000\ ug/mg) \qquad \text{Equation A1-8}$$

Review of Toxicity Data for Specific Chemicals

Below are reviews of toxicity data for some of the chemicals in DRAS. The reviews below explain the reasoning behind whether route-to-route extrapolations were used in some instances and the reasoning behind toxicity value selection in DRAS that is different from the hierarchy selection process described previously in this section.

Arsenic

1) The listed DRAS values for CSF_O and RfD_O are correct values based on IRIS.

2) An IUR value of 4.3E-03 $(ug/m^3)^{-1}$ is found in IRIS, and we used this value to calculate a CSF_I of 15 $(mg/kg\text{-}day)^{-1}$. Since this is the same as the listed DRAS value, no change was necessary.

3) Note: IRIS has only one set of toxicity factors for Arsenic. These should be applied to analytical data for Ar(III), Ar (V) or Total Arsenic. For purposes of evaluating arsenic risk, EPA generally evaluates arsenic risk as Total arsenic unless a specific regulation spells out how arsenic should be analyzed and reported. If the DRAS program directs petitioners to report results for Ar(III) and Ar (V), there is still only one set of toxicity factors available.

4) CalEPA has published an RfC value (chronic inhalation REL) of 0.015 $\mu g/m^3$ which was also listed in the RSL tables as the RfC value for arsenic. This RfC value is listed in DRAS.

Benzo(k)fluoranthene

1) The listed DRAS CSF_O value of 0.01 $(mg/kg\text{-}day)^{-1}$ is correct based on use of the Relative Potency Factor (RPF) factor approach (U.S. EPA 1993a) based on the IRIS CSF_O for Benzo(a)pyrene (U.S. EPA 2017).

2) The listed DRAS CSF_I of 0.02 $(mg/kg\text{-}day)^{-1}$ is the result of applying the RPF factor approach based on the U.S. EPA IRIS CSF_I for Benzo(a)pyrene (U.S. EPA 2017).

Benzo(a)anthracene

The currently listed DRAS values are correct. The listed CSF_I of 0.2 $(mg/kg\text{-}day)^{-1}$ and the listed CSF_O of 0.1 $(mg/kg\text{-}day)^{-1}$ are acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Benzo(b)fluoranthene
The currently listed DRAS values are correct. The listed CSF_I of 0.2 $(mg/kg\text{-}day)^{-1}$ and the listed CSF_O of 0.1 $(mg/kg\text{-}day)^{-1}$ are acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Chlordane

IRIS states that the toxicology studies used to derive the toxicity factors were performed by administering Technical grade Chlordane to animals for both the oral and inhalation exposure routes. IRIS gives a definition of Technical grade Chlordane. Therefore, if the petitioner performs an analysis for Technical grade Chlordane or some other form of Chlordane, there is only one set of toxicity factors.

Chloroethane (Ethyl Chloride)

1) An RfC value of 10 $(mg/m^3)$is found in IRIS.

2) The listed DRAS RfD value is a subchronic PPRTV.

3) The oral cancer slope factor could not be verified and a superseded document from NCEA did not match with R9's estimates of the inhalation slope factor, therefore we do not recommend that the carcinogenic toxicity factors be left blank at this time.

Chloroform

1) When the IRIS file for chloroform was revised (Oct. 2001), EPA made a significant change in its interpretation of the toxicological evidence. In particular, IRIS determined that ingested chloroform acts by non-linear Mode of Action – chloroform must induce cytotoxicity as a prerequisite for the induction of tumors in rodents. In addition, at dose levels below the oral RfD, chloroform does not induce the level of

cytotoxicity and regenerative hyperplasia needed to induce the tumorigenic response. Therefore, the RfD was determined to be an adequate dose benchmark for cancer prevention. The following is the explanation found in the IRIS file:

> In the case of chloroform, the mode of action of carcinogenicity is reasonably well understood. Available data indicate that chloroform is not strongly mutagenic and chloroform is not expected to produce rodent tumors via a mutagenic mode of action (ILSI, 1997). Rather, there is good evidence that carcinogenic responses observed in animals are associated with regenerative hyperplasia that occurs in response to cytolethality (ILSI, 1997; U.S. EPA, 1998a,b). Because cytolethality occurs only at exposure levels above some critical dose level, a nonlinear approach is considered the most appropriate method for characterizing the cancer risk from chloroform.
> The Proposed Guidelines for Carcinogenic Risk Assessment (U.S. EPA, 1996) state that when the mode-of-action analysis based on available data indicates that the carcinogenic response is secondary to another toxicity that has a threshold, the margin-of-exposure analysis performed for toxicity is the same as is done for a noncancer endpoint, and an RfD for that toxicity may be considered in the cancer assessment. For chloroform, available evidence indicates that chloroform-induced carcinogenicity is secondary to cytotoxicity and regenerative hyperplasia; hence, the Agency relies on a nonlinear dose-response approach and the use of a margin-of-exposure analysis for cancer risk. The Agency has also chosen not to rely on a mathematical model to estimate a point of departure for cancer risk estimate, because the mode of action indicates that cytotoxicity is the critical effect and the reference dose value is considered protective for this effect.
>
> For more discussion of margin of exposure (MOE), see the Toxicological Review for Chloroform. Based on the kidney tumor of the drinking water study (Jorgenson et al., 1985), a point of departure (Pdp or LED10) of 23 mg/kg/day can be calculated using quantitative modeling of tumor dose-response data. Comparing the Pdp to the RfD of 0.01 mg/kg/day leads to a MOE of 2,000, which is considered large. Thus, in this case, the RfD for noncancer effect is also considered adequately protective of public health for cancer effects by the oral route, on the basis of the nonlinear dose response for chloroform and the mode of action for both cancer and noncancer effects having a common link through cytotoxicity.

We concluded that the existing CSF_O for chloroform be deleted and the Cal EPA cancer slope factor should not be adopted.

2) The listed DRAS CSF_I value should be rounded off to 0.081 $(mg/kg\text{-}day)^{-1}$.

3) The listed DRAS RfD_O value from IRIS is acceptable to use.

4) The 2020 RSLs lists a value derived from ATSDR. An RfC of 9.8E-02 (mg/kg day) was derived from a chronic inhalation MRL published by ATSDR in 1997.

Chromium

1) For Cr(III), CASRN 16065-83-1, IRIS states that the following factors cannot be developed: RfC (RfD_I), CSF_O, and IUR (CSF_I); Therefore, for Cr(III), DRAS lists only an RfD_O of 1.5 (mg/kg-day).

2) For Cr (VI), CASRN 18540-29-9, the listed DRAS RfD_O is correct;

3) IRIS identifies an RfC of 8E-06 (mg/m^3) for exposure to mists and aerosols (such as that emitted from chromium plating operations) and an RfC of 1E-04 (mg/m^3) for exposure to a release of Cr(VI) particulates. The RfC used in DRAS is 1E-04 (mg/m^3) since the primary exposure scenario in DRAS for inhalation of chromium is via particulate release from the surface of a landfill.

4) For Cr (VI), the IRIS IUR is 1.2E-02 $(ug/m^3)^{-1}$ and the calculated CSF_I from the IUR is 42 $(mg/kg\text{-}day)^{-1}$. As stated in IRIS, industrial worker exposure was known to be from Cr(VI)-Cr(III) mixtures, so there is some uncertainty in the actual slope factor that would be due to Cr(VI) alone. The Cr(VI):Cr(III) ratio was assumed to be at least 1:6 for development of the slope factor; therefore, the highest possible CSF_I would be $7 \times 42 = 2.9E+02$ $(mg/kg\text{-}day)^{-1}$. Therefore, we used this latter value to evaluate exposure to Cr(VI)

A separate DRAS constituent, Chromium, CASRN 7440-47-4, included in previous versions of DRAS to evaluate mixtures of Cr(III) and Cr(VI), was removed from the database because of the difficulty in assigning or weighting chemical parameter values that are widely different between the two species, Cr(III) and Cr(VI). Since any chromium present is highly likely to be comprised of either Cr(III), Cr(VI), or both species, EPA recommends determining the concentration of Cr(VI) in the waste and subtracting it from the total chromium concentration to obtain values of both chromium species. Alternatively, the total chromium concentration can be assumed to be entirely the Cr(VI) species which will result in a conservative calculation in DRAS based on its higher toxicity and mobility.

Chrysene

The currently listed DRAS values are correct. The listed CSF_I of 0.002 $(mg/kg\text{-}day)^{-1}$ and the listed CSF_O of 0.001 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Dibenz(a,h)anthracene

The currently listed DRAS values are correct. The listed CSF_I of 2 $(mg/kg\text{-}day)^{-1}$ and the listed CSF_O of 1 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

1,1-Dichloroethane

1) The listed HEAST RfC value of 0.5 (mg/m^3) is correct and is the only provisional toxicity factor available until the IRIS file is revised.

2) The EPA Region 9 PRG reference from 2004 originally recommended a route-to-route extrapolation for RfD. However, EPA Superfund has since provided a provisional RfD_O under PPRTV and that value is used as the default in DRAS.

3) There are no acceptable cancer slope factors available for this chemical. We suggest not using the CalEPA listed slope factors that were derived from an NCI 1977 study in rats. The EPA IRIS program re-evaluated this study and determined that it contained too many confounding results to use for deriving a CSF_O value.

Dichloropropene (cis-, trans-, mixture)

In the "mixture" heading, all of the listed DRAS values are correct except for the RfD_I. Since the IRIS RfC value is 0.02 (mg/m^3), the calculated DRAS RfD_I should be 0.00571 (mg/kg-day);

HCH and Lindane

For the RfD_I, we assume that route-to-route extrapolation from oral exposure is valid, and use the values listed in the PRG column as the values to adopt for DRAS.

Indeno(1,2,3-cd)pyrene

The currently listed DRAS values are correct. The listed CSF_I of 0.2 $(mg/kg\text{-}day)^{-1}$ and the listed CSF_O of 0.1 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Lead

There are no IRIS cancer slope factors or Reference Doses for lead. EPA bases the protective media concentration on an uptake-absorption model in children up to seven years old in the child model; and for a pregnant woman in the adult model (to provide protection to the adult and the unborn child).

The general cleanup program policies are: lead releases to residential soil should not cause total soil lead concentration to exceed 400 (mg/kg); lead releases to industrial/commercial use soil (i.e., adult only exposure) should not cause total soil concentration to exceed 800 (mg/kg);

Mercury

1) The CASRN of 7439-97-6 means Hg(0) or elemental mercury. The listed DRAS RfD_I value and RfC value are correct however, there is no RfD_O value for Hg(0), so it is not appropriate to use the value from methyl mercury.

2) Mercury and compounds: This for the inorganic Hg valence states above zero, including Hg(II), such as HgCl2 and HgO. The only available toxicity factor is the RfD_O of 0.0003 (mg/kg-day).

3) Methyl mercury: This is for organic mercury that has accumulated and bioconcentrated in organic tissues (e.g., fish, wildlife). The only available toxicity factor is the RfD_O of 0.0001 (mg/kg-day). This constituent is not easy to measure accurately in tissues. So the default assumption is that all mercury detectable in organic tissues is methyl mercury;

4) DRAS currently includes separate constituents of concern for mercury and methyl mercury due to the differences in both toxicity and fate and transport in the environment. Methyl mercury is listed as *Mercury (Fish Pathway Only)* while all other forms of mercury are evaluated under *Mercury.*

Nickel

1) The CASRN of 7440-02-0 is for nickel salts or nickel compounds. The listed DRAS RfD_O of 0.02 (mg/kg-day) should be used for ingestion of all forms of nickel except nickel subsulfide as explained below.

2) Use the listed IRIS value of 0.84 (mg/kg-day) $^{-1}$ for inhalation (CSF_I) of all forms of nickel except nickel subsulfide as explained below. We did not assume route-to-route extrapolation to derive a CSF_O value.

Polychlorinated biphenyls (PCBs) (Aroclors)

In most PCB analyses performed by the historical EPA method, the results are presented as an amount of total Aroclors and/or amounts of specific Aroclors (1254, 1260, 1248, etc.). This gives very little information about the actual level of chlorination in the mixture. So when Aroclor analysis is performed, assume that the mixture is highly chlorinated and use the "high risk" slope factors: $CSF_O = 2$ (mg/kg-day) $^{-1}$; and $CSF_I = 2$ (mg/kg-day) $^{-1}$.

For non-cancer hazard, assume that the mixture is composed of the most hazardous Aroclor (1254) and use the $RfD_O = 0.00002$ (mg/kg-day). In this case, it is acceptable to use route-to-route extrapolation and apply an RfD_I value of 0.00002 (mg/kg-day) because of evidence that inhalation exposure of PCBs can result in adverse effects at distant sites from the lung.

To apply the "low risk" toxicity factors, the petitioner needs to perform a more refined sample analysis. For example, to obtain evidence for a low risk mixture, GC-MS analysis needs to be performed to accomplish an isomer group analysis that will report the results as mono- through deca- PCB homologs. This will yield more specific data about the chlorine content of the mixture. Then IRIS states that the mixture should be assumed to be low risk only if "congener or isomer analyses verify that congeners with more than 4 chlorines comprise < 0.5% of the total PCBs." And by analogy, only apply the highest RfD_O of 0.00007 (mg/kg-day) if analysis shows that the chlorine content is very low or if the mixture can be verified to be composed of only Aroclor 1016.

Trichlorophenol, 2,4,6-

1) DRAS should use the listed IRIS values for CSF_O, 0.011 (mg/kg-day)$^{-1}$, and CSF_I, 0.011 (mg/kg-day)$^{-1}$.

2) DRAS should use the NCEA provisional value for RfD_O. Also, we used route-to-route extrapolation of the NCEA RfD_O to obtain the RfD_I because IRIS used route-to-route extrapolation to obtain the IUR from the CSF_O.

Vinyl Chloride

IRIS has several values listed for CSFO and CSFI. Lowest value was used in DRAS which is the same value listed in RSL table.

Evaluation of Whether to Retain Route-to-Route Extrapolations from DRAS3 to DRAS4

Acetophenone; CASRN 98-86-2

Acetophenone has an RfD value listed in its IRIS profile. The RfD is based on a No Observed Adverse Effects Level in a subchronic oral administration study in rats. This was a single subchronic study that reported no effects on growth, hematologic parameters, or histopathology of tissues. The IRIS profile does not report on any studies of inhalation exposure studies in humans or animals. There is a PPRTV profile for Acetophenone (EPA/690/R-11/002F Final 06-15-2011) that is more recent than the IRIS profile and reports on some more recent exposure studies than those described in the IRIS entry. For the oral route of exposure, no additional adequate studies were reported that could update the original RfD

value or allow derivation of a new provisional p-RfD value. For the inhalation route, a few studies were identified on inhalation exposure in humans and lab animals. The only significant observations in animal studies were avoidance reactions to acetophenone and changes in the histopathology of the olfactory bulb of the respiratory tract. The studies were not adequate to derive a provisional p-RfC value. However, the observations of inhalation avoidance and potential changes in the olfactory bulb are consistent with suspecting that Acetophenone could be respiratory irritant in animals and humans.

Conclusion – Do Not use route-to-route extrapolation.

Antimony; CASRN 7440-36-0

This inorganic constituent has an IRIS profile. IRIS documents an RfD value based on the findings of reduced life span and decreased circulating glucose and cholesterol levels in rats. Data were insufficient to derive an RfC value. The ATSDR has published a Toxicological Profile of this chemical. ATSDR found studies linking inorganic antimony exposure to multiple exposure routes and potential target organs. For inhalation exposure, ATSDR concluded that antimony is presumed to cause respiratory effects following inhalation exposure based on low evidence in workers exposed to antimony oxides and a high level of evidence in several animal species exposed to antimony trioxide, antimony trisulfide, and antimony ore. The respiratory effects include irritation of epiglottis epithelium, increases in the number of alveolar/bronchiolar macrophages, decreases in lung clearance, and lung interstitial fibrosis. Consequently, inhaled antimony is likely to result in direct lung/respiratory effects which could influence absorption from the lungs.

Conclusion: Do Not use route-to-route extrapolation.

Benzaldehyde; CASRN 100-52-7

Benzaldehyde has an RfD value listed in an IRIS entry. The RfD is based on a No Observed Effects Level in a subchronic oral administration studies in rats and mice. These studies reported effects described as kidney tubular necrosis and forestomach cell hyperplasia. The IRIS profile does not report on any studies of inhalation exposure studies in humans or animals.

There is a PPRTV profile for Benzaldehyde (EPA/690/R-15/001F Final 11-12-2015) that is more recent than the IRIS profile and reports on some more recent exposure studies than those described in the IRIS entry. This updated evaluation of benzaldehyde reported on a short-term inhalation study in rats. This short-term exposure study of benzaldehyde inhalation exposure reported histopathological changes in nasal epithelium, including goblet cell metaplasia in males and mild morphological changes in females. In addition, peripheral extrarespiratory tract effects were found in some of the same animals, including increased liver weights and changes in red and white blood cell counts. These findings from a single study were not adequate to derive a provisional p-RfC. However, these effects indicate that benzaldehyde can exert adverse effects in the respiratory tract and that possible adverse effects outside the respiratory tract are different from those associated with oral exposure because they could affect a different organ system or mechanism of action.

Conclusion – Do Not use route-to-route extrapolation.

Bis(2-chloroisopropyl) ether; CASRN 39638-32-9; Bis(2-chloro-1-methylethyl) ether

This chemical has an IRIS profile listed under its synonym name: Bis(2-chloro-1-methylethyl) ether. IRIS documents an RfD value based on decrease in hemoglobin and possible erythrocyte destruction in

mice. The RfD value is listed as 4E-02 mg/kg-day. Data were insufficient to derive an RfC value. The ATSDR has not published a Toxicological Profile of this chemical and a PPRTV entry could not be located. No reliable information could be located on the possible inhalation effects of this chemical to rule out direct irritant effects or direct respiratory tract toxic effects.

Conclusion: Do Not use route-to-route extrapolation.

Bis(2-Chloroethoxy) methane; CASRN 111-91-1

This chemical does not have an entry in IRIS. There is a PPRTV profile for Bis(2-Chloroethoxy) methane (EPA/690/R-06/005F Final 9-22-2006). One subchronic study of oral administration of bis(2-chloroethoxy)methane to rats was located: a 90-day oral gavage study conducted by Bio/Dynamics (1990a), wherein Sprague-Dawley rats (10/sex/dose group) received oral doses of 0, 10, 20, 40, 80, or 120 mg/kg-day of bis(2-chloroethoxy)methane in corn oil. Subchronic and chronic oral provisional p-RfDs for bis(2-chloroethoxy) methane were derived using a NOAEL/LOAEL approach, based on liver lesions (centrilobular hepatocellular hypertrophy) in male rats receiving 20 mg/kg-day or more of bis (2-chloroethoxy) methane. This study identified a NOAEL of 10 mg/kg-day for the critical effect. The finding that the liver is a sensitive target for bis(2-chloroethoxy) methane is supported by the short-term range-finding study (Bio/Dynamics, 1990b). For the rat NOAEL of 10 mg/kg-day for liver lesions established by Bio/Dynamics (1990a), a combined uncertainty factor of 300 was applied. The uncertainty factors included a 10 for interspecies extrapolation, a 10 for human variability, and a 3 for database deficiencies (including lack of reproductive and developmental toxicity tests), resulting in a combined uncertainty factor of 300. A provisional subchronic oral p-RfD of 0.03 mg/kg-day was calculated. A provisional chronic oral p-RfD was also be derived by dividing the NOAEL of 10 by a combined uncertainty factor of 3000. The uncertainty factors included a 10 for extrapolation from a subchronic study, a 10 for interspecies extrapolation, a 10 for human variability, and a 3 for database deficiencies, resulting in a combined uncertainty factor of 3000. A provisional chronic oral p-RfD of 0.003 mg/kg-day was calculated.

No reports were located regarding the subchronic or chronic toxicity of bis(2-chloroethoxy)methane in humans or animals by inhalation exposure. Consequently, information is not available to determine if the chemical has respiratory tract irritant effects or extra-respiratory adverse effects from inhalation and absorption of the chemical in the vapor phase.

Conclusion – Do Not use route-to-route extrapolation.

Cyanide; CASRN 57-12-5

This inorganic constituent has a revised IRIS profile which was published in 2010 along with a formal toxicological report (TOXICOLOGICAL REVIEW OF HYDROGEN CYANIDE AND CYANIDE SALTS). The IRIS profile documented an RfD value based on the findings of decreased cauda and whole epididymis weights, decreased testes weight, and altered sperm parameters in rats. The form of cyanide administered orally to study rats was NaCN in water. For the inhalation route of exposure, a vapor phase form of cyanide is the prime concern. Studies of subacute inhalation exposure of industrial workers to HCN showed that thyroid enlargement and altered iodide uptake were designated as the critical effects. EPA calculated an RfC based on thyroid enlargement and altered iodide uptake reported in an occupational study of electroplating workers which is supported by other occupational studies. After adjustment of the Lowest Observed Adverse Effects Level for continuous exposure and appropriate Uncertainty Factors, a recommended RfC value of 8E-04 mg/m3 was derived.

Conclusion: Do Not use route-to-route extrapolation; Use the RfC value described above.

DDD; CASRN 72-54-8

DDD has a p-RfD value listed as a PPRTV entry (EPA/690/R-17/006 FINAL 09-20-2017). The RfD is based on the finding of liver lesions in male and female rats.
ATSDR has published a Toxicological Profile for DDD and the two closely related structural isomers, DDT and DDE, as a general class of chemicals.
(https://www.atsdr.cdc.gov/ToxProfiles/tp.asp?id=81&tid=20). ATSDR did not find any studies showing specific direct respiratory effects of DDD in workers who could have experienced inhalation exposure. And available studies did not provide evidence that DDD and its isomers are direct respiratory irritants or cause portal of entry effects in the lung. Therefore, absorption of DDD or its isomers could occur after inhalation without causing significant lung or respiratory track irritation effects or metabolism in the lung.

Conclusion - Retain use of route-to-route extrapolation.

Diazinon; CASRN 333-41-5
Dimethoate; CASRN 60-51-5
Disulfoton; CASRN 298-04-4
Malathion; CASRN 121-75-5
Sulfotep; CASRN 3689-24-5

As a group, all of the above constituents cause their primary biological effect and non-cancer effect by inducing decreased cholinesterase activity, and the chemicals are known as cholinesterase inhibitors. Based on their known pharmacological activity, cholinesterase inhibitors can exert their activity peripheral to the lungs very rapidly following inhalation exposure with only minimal direct lung tissue irritation from chronic exposure.
(https://www.atsdr.cdc.gov/csem/cholinesterase/docs/cholinesterase.pdf).
It would be appropriate to retain use of the RTRE procedure.

Conclusion - Retain use of route-to-route extrapolation.

Dinitromethylphenol (2-Methyl-4.6-Dinitrophenol); (4,6-Dinitro-o-cresol) CASRN 534-52-1

This chemical does not have an IRIS entry. There is a PPRTV profile under the name 4,6-Dinitro-o-cresol (EPA/690/R-10/012F Final 4-22-2010). Along with other Dinitrocresols (DNOC), this chemical was used in the 1930's a weight loss drug which elevated basal metabolism activity. Side effects included headaches, lethargy, sweating, and loss of appetite. On a dose basis, humans were more sensitive to the adverse side effects than animals. Using the human data, the combined effects of weight loss, fatigue, and elevated basal metabolism weight were used to determine a LOAEL of 0.8 mg/kg-day. After application of appropriate Uncertainty factors, a provisional subchronic RfD of 8E-04 mg/kg-day was derived. However, the data were not considered appropriate to derive a provisional chronic p-RfD because a total Uncertainty Factors greater than 10,000 would be required. Instead, the Appendix of the report suggests the possible use of a screening level s-RfD value of 8E-05 mg/kg-day. No reports of reliable inhalation studies were located that could be used to identify any adverse health effects due to inhalation.

ATSDR has published a toxicological profile for Dinitrophenols (DNPs). And Dintromethylphenol is considered to be a member of that group because of similar structure and uses as a weight loss agent with

similar adverse side effects after human exposure. Reports of inhalation exposure effects to Dinitrophenols are limited but informative. Inhalation exposure of workers in chemical plants at relatively high concentrations reported health effects that included elevated body temperature, profuse sweating, and fatigue. These reports indicate that absorption is possible after DNP inhalation and that the gross adverse peripheral side effects following inhalation are quite similar to those seen for oral absorption. It is reasonable to conclude that inhalation exposure to Dinitromethylphenol would result in the same effects.

Conclusion: Retain the use of route-to-route extrapolation.

Dinitrotoluene 2,4- CASRN 121-14-2; Dinitrotoluene 2,6- CASRN 606-20-2

These two chemicals may be considered together because they are typically encountered in industry as a product containing a mixture of isomers that contain 2,4 and 2,6-DNT. And they are usually detectable a mixture of DNT isomers and waste sites and in waste material.

Where possible, EPA has summarized the toxicological effects of the individual isomers. The IRIS has a profile for 2,4-DNT which gives an oral RfD. The PPRTV data base a profile for 2,6-DNT. EPA suggested that a chronic screening oral s-RfD could be used for this isomer.

No studies were identified that could be used to derive provisional inhalation p-RfCs for 2,6-DNT or 2,4-DNT. Available epidemiological studies consist primarily of occupational studies in which workers were exposed to the technical grade DNT mixture, which consists primarily of the 2,4-DNT isomer. In these studies, dermal as well as inhalation exposure were investigated, and exposure to 2,6-DNT was not quantified. No animal inhalation studies are available for 2,6-DNT. The available data do not support derivation of any provisional or screening level RfC inhalation toxicity values.
ATSDR has published a toxicological profile for Dinitrotoluenes (DNTs). In general, the low vapor pressure of DNTs makes vapor phase exposure unlikely. No studies were found which documented systemic peripheral non-respiratory effects from situations where human inhalation exposures were possible in workplaces. One short-term study of 2.6-DNT inhalation exposure to rats showed evidence of lung congestion, suggesting that vapor phase DNTs are respiratory irritants.

Conclusion – Do Not use route-to-route extrapolation.

Di-n-octylphthalate; CASRN 117-84-0

This chemical does not have an IRIS entry. There is a PPRTV profile (EPA/690/R-12/023F Final 12-20-2012). The profile describes the lack of direct exposure studies in humans. Two chronic exposure studies of oral administration of the chemical in male rats were reported. The critical adverse effects were all hepatic effects characterized specifically as hepatocellular hypertrophy leading to hepatocellular degeneration and necrosis. The critical effect for defining the LOAEL was cytoplasmic liver vacuolation. The LOAEL was used to derive both a subchronic provisional p-RfD and a chronic provisional p-RfD. For inhalation exposure, no adequately described studies of Di-n-octylphthalate exposure to humans or animals are available.

ATSDR has published a toxicological profile for Di-n-octylphthalate. No studies were located on inhalation exposure of this chemical in humans or animals and no information is available on acute or subchronic peripheral systemic effects from inhalation exposure. Consequently, the available information is inadequate to characterize the chemical as a respiratory irritant or to determine if absorption from the respiratory tract could be expected.

Conclusion – Do Not use route-to-route extrapolation.

Diphenylamine; CASRN 122-39-4

A chronic oral RfD of 2.5E-02 mg/kg-day for diphenylamine is included in the IRIS database (2010). This value is based on decreased body-weight gain and increased liver and kidney weights in dogs in a 2-year feeding study. However, no RfC or cancer assessment is available on IRIS.

There is a PPRTV profile (EPA/690/R-11/026F Final 5-11-2011). In regard to providing an updated provisional p-RfD to possibly replace the IRIS RfD value, the PPRTV profile stated that additional studies that may be relevant have been discovered. These studies are summarized in this PPRTV assessment. However, these additional studies do not provide a lower or more credible Point of Departure than the study formerly used by IRIS. Also, the PPRTV report stated that effects of inhalation exposure to diphenylamine on animals have not been evaluated in subchronic or chronic duration, developmental, reproductive, or carcinogenic studies. ATSDR has not published a toxicological profile for Diphenylamine so additional information on inhalation exposure was not reported.

EPA's OPPTS Program performed a risk assessment for uses of diphenylamine as a post-harvest preservative for pears and apples (https://iaspub.epa.gov/apex/pesticides/f?p=HHBP:home) The report concluded that the low vapor pressure of the chemical means that evaporation and inhalation exposure would be negligible for applicators and handlers. No respiratory inhalation effects of the chemical were reported.

Based on the above information, it is likely that diphenylamine is not a respiratory irritant and may not have sufficiently volatility to be an inhalation concern. And there is significant uncertainty on the possibility that diphenylamine could be absorbed from the respiratory track.

Conclusion – Do Not use route-to-route extrapolation.

Hexahydro-1,3,5-trinitro-1,3,5-triazene (RDX); CASRN 121-82-4

This chemical commonly known as RDX has a revised IRIS profile published in 2018. IRIS documents an RfD value based on nervous system effects in rats. Data were insufficient to derive an RfC value, but the IRIS profile stated that inhalation exposure was a likely route for some persons exposed to RDX at production sites or waste sites. The ATSDR has published a Toxicological Profile of this chemical. The ATSDR described four studies of human exposure for which inhalation was the route of exposure that resulted in systemic peripheral (non-respiratory) effects with no reports of significant respiratory system direct effects or irritant responses.

Conclusion - Retain use of route-to-route extrapolation.

Isobutyl alcohol; CASRN 78-83-1

For this chemical, there no evidence of direct lung toxicity by chronic inhalation exposure.
And there is no significant evidence of respiratory tract irritant action at typical environmental exposure levels (See PPRTV entry for Isobutyl alcohol EPA/690/R-02/010F Final 5-31-2002).

There is evidence of peripheral systemic effects of isobutanol exposure. Isobutanol inhalation exposure was associated with hematological and CNS depression (non-respiratory effects) in animal exposure studies (See PPRTV entry for Isobutyl alcohol EPA/690/R-02/010F Final 5-31-2002).

Conclusion - Retain use of route-to-route extrapolation.

Methoxyclor; CASRN 72-43-5

ATSDR has published a Toxicological Profile on this insecticide. ATSDR did not find any studies showing specific direct respiratory tract effects of DDD in persons who could have experienced inhalation exposure. And available studies did not provide evidence that Methoxyclor is direct respiratory irritant or causes portal of entry effects in the lung. Therefore, absorption of Methoxyclor could occur after inhalation without causing significant lung or respiratory track irritation effects or metabolism in the lung.

Conclusion - Retain use of RTRE

Methylnapthalene 2- ; CASRN 91-57-6

This chemical has an IRIS profile. The IRIS chronic RfD (U.S. EPA, 2003) was based on a BMDL05 of 3.5 mg/kg-day for 5% extra risk of pulmonary alveolar proteinosis in male and female mice exposed to 2-Methylnaphthalene in the diet for 81 weeks (Murata et al., 1997). The IRIS profile did not describe any inhalation studies in humans or animals.

ATSDR has published a toxicological profile for Naphthalenes as a related chemical group. Based on three available studies, the nose is the most sensitive toxicity target in rats and mice following chronic inhalation exposure to naphthalene. Chronic inhalation exposure resulted in increased incidences of nonneoplastic and neoplastic lesions in the nose of rats (Abdo et al. 2001; Long et al. 2003; NTP 2000), nonneoplastic lesions in the nose of mice (NTP 1992a), and neoplastic and nonneoplastic lesions in the lungs of mice (NTP 1992a). No exposure-related lesions were found in other tissues or organs in these studies, which included comprehensive histopathological examinations of major tissues and organs. Nearly all mice of both sexes (>95%) exposed to naphthalene vapors for 2 years (10 or 30 ppm) showed chronic inflammation and metaplasia of the olfactory epithelium and hyperplasia of the nasal respiratory epithelium (NTP 1992a). Chronic lung inflammation was also observed in exposed mice, but at lower incidences than incidences for nasal lesions. Incidences for chronic lung inflammation were 0/70, 21/69, and 56/135 for male mice and 3/69, 13/65, and 52/135 for female mice exposed to 0, 10, or 30 ppm. In addition, exposure to 30 ppm (but not 10 ppm) increased the incidence of benign lung tumors (alveolar/bronchiolar adenomas) in female mice, compared with controls. In rats of both sexes, inhalation of 10, 30, or 60 ppm naphthalene induced nonneoplastic and neoplastic lesions only in the nasal cavity (Abdo et al. 2001; NTP 2000). Nearly all rats in each exposure group (> 95%) showed nonneoplastic nasal lesions. Nonneoplastic nasal lesions in exposed rats included (1) hyperplasia, atrophy, chronic inflammation, and hyaline degeneration of the olfactory epithelium and (2) hyperplasia, metaplasia, or degeneration of the respiratory epithelium or glands. Neoplastic lesions associated with naphthalene exposure in rats were olfactory epithelial neuroblastoma and respiratory epithelial adenoma.

The above description for the direct respiratory effects of napthalene by inhalation can reasonably be extrapolated to inhalation exposure by 2-methylnaphthalene. The results are also consistent with the conclusion that naphthalenes act directedly on the respiratory system and the resulting long-term exposure effects are different and likely act by a different mechanism than the systemic effects due to chronic oral exposure.

Conclusion – Do Not use route-to-route extrapolation.

Methyl parathion; CASRN 298-00-0

This chemical has an IRIS profile. Methyl parathion is a chemical which acts as cholinesterase inhibitor. According to the IRIS profile, in a subchronic study with methyl parathion in humans, Red Blood Cell (RBC) cholinesterase depression was reported, with a NOAEL of approximately 0.3 mg/kg/day. ATSDR has published a toxicological profile for methyl parathion. ATSDR reported that accidental exposure in children by oral, dermal, or inhalation exposure all caused cholinesterase depression characterized by signs and symptoms of lethargy, increased salivation, and increased respiratory secretions.

Based on their known common pharmacological activity, cholinesterase inhibitors as a pesticide group can exert their activity peripheral to the lungs very rapidly following inhalation exposure with only minimal direct lung tissue irritation from chronic exposure.
https://www.atsdr.cdc.gov/csem/cholinesterase/docs/cholinesterase.pdf).

Conclusion - Retain use of route-to-route extrapolation.

Methylene Bromide; Dibromomethane; CASRN 74-95-3

There is no evidence of direct lung toxicity by chronic inhalation exposure.
There is no significant evidence of respiratory tract irritant action at typical environmental exposure levels. (See PPRTV entry for Methylene Dibromide EPA/690/R-09/031F Final 9-30-2009.)

There is evidence of peripheral systemic effects of Methylene Bromide exposure. A single Methylene Bromide inhalation study of exposure was found to be associated with non-respiratory effects in a single study. The effect was an increase in Carboxyl Hemoglobin levels in blood that were likely the result of liver metabolism (See PPRTV entry for Methylene Dibromide EPA/690/R-09/031F Final 9-30-2009). Based on the Carboxyl Hemoglobin study, the PPRTV Report recommended assigning a Screening Level RfC of 4.0E-03 mg/m3 (See PPRTV entry for Methylene Dibromide EPA/690/R-09/031F Final 9-30-2009).

Conclusion – Do not use route-to-route extrapolation; Use the PPRTV Screening Level RfC of 4.0E-03 mg/m3 mentioned above.

Nitro-o-toluidine; 2-Methyl-5-Nitroaniline; CASRN 99-55-8

There is no evidence of direct lung toxicity by chronic inhalation exposure.
There is no significant evidence of respiratory tract irritant action at typical environmental exposure levels (See PPRTV entry for 2-Methyl-5-Nitroaniline EPA/690/R-11/035F Final 3-31-2011).

There is some evidence of peripheral systemic effects of exposure. 2-Methyl-5-Nitroaniline exposure from a likely inhalation route was associated with liver damage and changes in liver enzyme levels in a single report about human exposure in an industrial workplace (See PPRTV entry for 2-Methyl-5-Nitroaniline EPA/690/R-11/035F Final 3-31-2011).

However, the PPRTV Report states the following finding:
“The only available data on human inhalation exposure to 2-methyl-5-nitroaniline is a single case study of an occupationally-exposed worker who developed fulminant hepatitis, and an observational study of a

small cohort of exposed workers who showed evidence of liver dysfunction following several weeks of working with the compound in a hair dye manufacturing facility. Quantitative estimates of exposure and adverse liver effects were not available for these workers. No animal studies investigating the effects of inhalation exposure have been conducted. Therefore, data are inadequate for the derivation of subchronic and chronic p-RfCs for 2-methyl-5-nitroaniline."

Apparently, there is no predictable relationship between the single acute industrial exposure report and chronic oral exposure studies in lab animals.

Conclusion – Do Not use route-to-route extrapolation.

Octamethyl Pyrophosphoramide; CASRN 152-16-9

The only EPA database resource for toxicity values on this chemical is the HEAST (HEAST 1997). The HEAST non-cancer endpoint is listed as Decreased Cholinesterase Activity. This chemical is known to act as a Cholinesterase Inhibitor. The RfD value is listed as 2E-03 mg/kg-day. Based on the known pharmacological activity, cholinesterase inhibitors can exert their activity peripheral to the lungs very rapidly following inhalation exposure with only minimal direct lung tissue irritation. (https://www.atsdr.cdc.gov/csem/cholinesterase/docs/cholinesterase.pdf). It would be appropriate to retain use of the route-to-route extrapolation procedure.

Conclusion - Retain use of route-to-route extrapolation.

Pronamide; CASRN 23950-58-5

Pronamide has an RfD value listed in an IRIS entry. The RfD is based on a Lowest Observed Effects Level for increased liver weight or body weight in a subchronic oral administration study in dogs. No information was located on the administration of Pronamide by the inhalation route of exposure in animal studies or human epidemiological studies. However, inhalation exposure to Pronamide can cause throat irritation and cause coughing and wheezing. https://nj.gov/health/eoh/rtkweb/documents/fs/1592.pdf). Consequently, Pronamide is likely a respiratory irritant by the inhalation route of exposure.

Conclusion: Do Not use route-to-route extrapolation.

Pyrene; CASRN 129-00-0

Pyrene has an RfD value listed in an IRIS entry. The RfD is based on the No Adverse Effects Level for renal tubular degeneration and kidney fibrosis in a subchronic oral administration study in mice. No direct inhalation studies of Pyrene were located for lab animal or human epidemiological studies. However, several human epidemiologic studies of polycyclic aromatic hydrocarbon mixtures (including Pyrene) exposure in industrial settings by the inhalation route have shown that peripheral systemic effects outside the lung have been documented. Those effects included effects on the immunologic and lymphoreticular cells and formation of DNA adducts in blood cells.

Conclusion - Retain use of route-to-route extrapolation.

Tetrachlorophenol - 2,3,4,6; CASRN 58-90-2

Tetrachlorophenol has an RfD value listed in an IRIS entry. The RfD is based on the No Adverse Effects Level for the elevation of liver and kidney organ weights and the finding of liver cell hypertrophy in rat studies. No direct inhalation studies of Tetrachlorophenol were located for lab animal or human epidemiological studies.

However, ATSDR has published a Toxicological Profile for Chlorophenols as a general class of chemicals (https://www.atsdr.cdc.gov/toxprofiles/tp.asp?id=941&tid=195). Chlorophenols have been widely used chemicals in industrial workplaces. ATSDR did not find any studies showing specific direct respiratory effects of chlorophenols in workers who could have experienced inhalation exposure. Workers who were exposed to trichlorophenol isomers, but not tetrachlorophenol isomers, experienced upper airway irritation or chest wheezing. These studies did not provide significant evidence that tetrachlorophenol is a direct respiratory irritant.

Conclusion - Retain use of route-to-route extrapolation.

Tin; CASRN 7440-31-5

This inorganic constituent does not have an IRIS profile. The ATSDR has published a Toxicological Profile of this chemical. The ATSDR evaluated the inhalation route of exposure and the available information on the effects of inorganic tin and organic tin ("organotin") from inhalation exposure. For inorganic tin: Stannic oxide dust or fumes produce a benign form of pneumoconiosis, known as stannosis in humans. The workers exhibiting this pulmonary condition had industrial exposures ranging from 15 to 20 years. Chest x-rays of the workers showed discrete opaque shadows throughout the lungs, attributed to stannic oxide deposits. However, there was no impairment of pulmonary function or systemic disease. For organotin: Tributyltin oxide has been implicated in producing irritation of the upper respiratory tract and chest irritation, tightness, and pain in workers using a rubber material containing tributyltin oxide. Exposure conditions were not described. No changes were observed in pulmonary function tests (NIOSH 1976). An accidental exposure report found that all members of a family of five (two adults and three children) complained of sore throat, burning nose, and wheezing 24 hours after a room in their home had been painted with a product containing tributyltin oxide for mildew control. In another report, cough and difficulty in breathing, characterized by inspiratory discomfort, were observed in a man a few hours after inhaling an unspecified amount of powdered trimethyltin chloride. Shortness of breath and chest discomfort was still present 20 days after the exposure. In lab animals, inflammatory changes consisting of hyperemia and bronchitis were observed in the respiratory system of rabbits exposed to 4–6 mg/m3 (0.30–0.45 ppm) tributyltin chloride for 95 days. Histopathology, consisting of severe bronchitis and vascular and alveolar edema, was seen in rats exposed to 2 mg tin/m3 (0.41 ppm) as a mixture of tributyltin bromide (0.39 ppm), dibutyltin dibromide (0.02 ppm), for 80 days (Iwamoto 1960). All of the above findings provide significant evidence that tin and organotin compounds are direct respiratory irritants and can induce direct respiratory tissue responses.

Conclusion: Do Not use route-to-route extrapolation.

Toxaphene; CASRN 8001-35-2

This pesticide has an IRIS profile. IRIS documents an Oral Cancer Slope factor and an Inhalation Unit Risk factor. IRIS determined that data were insufficient to derive an RfD value. There is no screening level p-RfD value available in the PPRTV data base.

Conclusion – Use of the route-to-route extrapolation procedure is not possible.

Trichlorophenoxypropionic acid- 2,4,5 (2,4,5-TP)]; Silvex CASRN 93-72-1

This pesticide has an IRIS profile. IRIS documents an RfD value based on histopathological changes in the liver of dogs. Data were insufficient to derive an RfC value. The ATSDR has not published a Toxicological Profile of this chemical and a PPRTV entry could not be located. No reliable information could be located on the possible inhalation effects of Silvex to rule out direct irritant effects or direct respiratory tract toxic effects.

Conclusion: Do Not use route-to-route extrapolation.

Trichlorophenoxyacetic Acid (2,4,5-T); CASRN 93-76-5

This pesticide has an IRIS profile. IRIS documents an RfD value based on increase in urinary excretion of coproporphyrins and mineralized in the renal pelvis of rats. Data were insufficient to derive an RfC value. The ATSDR has not published a Toxicological Profile of this chemical and a PPRTV entry could not be located. No reliable information could be located on the possible inhalation effects of 2,4,5-T to rule out direct irritant effects or direct respiratory tract toxic effects.

Conclusion: Do Not use route-to-route extrapolation.

Trinitrotoluene-2,4,6; CASRN 118-96-7
This explosive chemical commonly known as TNT has an IRIS profile. IRIS documents an RfD value based on liver effects in dogs which included microscopic evidence of liver cirrhosis and macroscopic evidence of hepatocyte cloudy swelling, hepatomegaly, and increase in liver weight. IRIS did not evaluate any studies on the inhalation route of exposure. The ATSDR has published a Toxicological Profile of this chemical. ATSDR reviewed several reports on inhalation exposure to TNT. Inhalation exposure at relevant workplace or environmental concentrations was associated with several systemic adverse effects including hematological effects, hepatic enzyme effects, and ocular effects. The hepatic effects reported in exposed humans were consistent with those observed in oral administration to TNT in dogs. These peripheral effects appeared to be manifested in the absence of accompanying effects directly on the respiratory system, and TNT was not reported to have significant respiratory irritant effects.

Conclusion - Retain use of route-to-route extrapolation.

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TABLE A-1-1

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)	Experimentally measured value (Lee et al. 2012).	3.78E-05
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
Log K_{ow} (unitless)	Hansch (1995)	3.92
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	7.60E-01
*t** (hr/event)	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)	5.61E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-1

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-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 72 kg.	2E-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

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

TABLE A-1-2

CHEMICAL-SPECIFIC INPUTS FOR ACENAPTHYLENE (208-96-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	152.20
T_m (K)	CRC Handbook (1995)	365.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Experimentally measured value (Bamford et al. 1999).	1.25E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.39E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.53E-06
Log K_{ow} (unitless)	Hansch (1995)	3.94
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.55E-01
t	τ value was obtained from U.S. EPA (1992b).	7.42E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	6.23E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	--	NA
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	NA
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND

TABLE A-1-2

CHEMICAL-SPECIFIC INPUTS FOR ACENAPTHYLENE (208-96-8)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-3

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

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)	Experimentally measured value (Ji and Evans 2007).	6.6E-05
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
Log K_{ow} (unitless)	TSCATS	-0.34
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	7.60E-01
*t** (hr/event)	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)	3.24E+-1

TABLE A-1-3

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	9E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA(2020b).	7.9E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	17

Notes: NA = Not applicable
ND = No data available

TABLE A-1-4

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)	Experimentally measured value (Poulain et al. 2010).	3.4E-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
Log K_{ow} (unitless)	Hansch (1995).	-0.24
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.	5.81E-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.	5.81E-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.	4.36E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.70E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.00E-01
*t** (hr/event)	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
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	4.00E-01

TABLE A-1-4

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

Parameter	Reference and Explanation	Value
	derived values obtained from various literature sources cited in U.S. EPA (1998)	
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	9E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	ATSDR MRL (ATSDR 2020).	3.1E+1
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	1.5E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-5

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)	Experimentally measured value (Hiatt 2013).	1.640E-05
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
Log K_{ow} (unitless)	Hansch (1995).	-0.34
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.	6.44E-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.	6.64E-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.	4.38E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	6.10E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.60E-01
*t** (hr/event)	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
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	Route to route extrapolation from RfC.	2E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-5

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	6E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-6

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)	Experimentally measured value (Hiatt 2013).	1.013E-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
Log K_{ow} (unitless)	Hansch (1995).	1.58
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.	3.58E+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.	3.58E-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.	2.68E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.10E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.70E-01
*t** (hr/event)	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)		9.35E+00

TABLE A-1-6

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

Parameter	Reference and Explanation	Value
	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)	
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-7

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)	Experimentally measured value (Snider and Dawson 1985).	1.4E-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
Log K_{ow} (unitless)	Hansch (1995).	-0.01
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.	1.18E+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.	1.18E-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.	8.82E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	8.50E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.90E-01
*t** (hr/event)	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)		5.79E-01

TABLE A-1-7

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

Parameter	Reference and Explanation	Value
	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)	
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-8

CHEMICAL-SPECIFIC INPUTS FOR ACRYLAMIDE (79-06-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	357.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	9.20E-06
S (g/100ml H_2O)	Geometric mean value cited in U.S. EPA (1994c).	2.15E+02
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	5.90E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.67
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.	3.53E-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-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.	2.65E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.40E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	5.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)		1.82E-01

TABLE A-1-8

CHEMICAL-SPECIFIC INPUTS FOR ACRYLAMIDE (79-06-1)

Parameter	Reference and Explanation	Value
	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)	
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5E-01
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	6E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	4E-01
MCL	National Primary Drinking Water Regulations.	1.00E+00 TT
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-9

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)	Experimentally measured value (Hiatt 2013).	8.343E-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
Log K_{ow} (unitless)	Hansch (1995).	0.25
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.	1.89E+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.	1.89E-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.	1.42E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.43E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.80E-01
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-9

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

Parameter	Reference and Explanation	Value
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)	HEAST (U.S. EPA 1997c).	1E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5.4E-01
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.4E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	7.6E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-10

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)	Experimentally measured value (Cetin et al. 2006).	4.92E-04
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
Log K_{ow} (unitless)	DeBruijn (1989).	6.5
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.50E+01
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-10

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

Parameter	Reference and Explanation	Value
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)	1.32E+06
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-05
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.7E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.8E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3E-01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-11

CHEMICAL-SPECIFIC INPUTS FOR ALLYL CHLORIDE (107-05-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	76.53
T_m (K)	Montgomery and Welkom (1991)	138.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.80E-01
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.40E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	7.540E-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).	1.08E-05
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	1.93
K_{oc} (mL/g)	K_{cw} value cited in U.S. EPA (1995g).	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.	2.02E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.80E-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).	1.73E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-11

CHEMICAL-SPECIFIC INPUTS FOR ALLYL CHLORIDE (107-05-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Route to route extrapolation from RfC.	3E-04
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020).	2.1E-02
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-03
Inhalation [1] *CSF* (mg/kg/day)$^{-}$	CalEPA (2020).	2.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-12

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)	Experimentally measured value (Altschuh et al. 1999).	1.9E-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
Log K_{ow} (unitless)	Hansch (1995).	0.9
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.	7.67E+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.	7.67E-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.	5.75E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.60E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.20E-01
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-12

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

Parameter	Reference and Explanation	Value
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+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	7E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5.7E-03
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-13

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.37E-02
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	6.23E-05
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
Log K_{ow} (unitless)	Hansch (1995).	4.45
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.07E+00
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-13

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

Parameter	Reference and Explanation	Value
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)	2.51E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-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 72 kg.	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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-14

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	45 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e).	45 at pH=6.8
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr/event)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b)	4.00E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-14

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-15

CHEMICAL-SPECIFIC INPUTS FOR ARAMITE (140-57-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	1.90E-07
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
Log K_{ow} (unitless)	U.S. EPA (2000).	4.82
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.	5.47E+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 organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.47E+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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.11E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	4.00E+01

TABLE A-1-15

CHEMICAL-SPECIFIC INPUTS FOR ARAMITE (140-57-8)

Parameter	Reference and Explanation	Value
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).	7.54E+03
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	5E-02
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.5E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	2E-01
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.6E-02
MCL	National Primary Drinking Water Regulations.	6E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Notes: NA = Not applicable
ND = No data available

TABLE A-1-16

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	74.92
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,091 at 36 atm
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.07E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.24E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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 (1998b)	1.14E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.5E+00

TABLE A-1-16

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	CalEPA (2020).	1.5E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.5E+01
MCL	National Primary Drinking Water Regulations.	1.0E-02
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.50E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-17

CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	Calculated value (Hilal et al. 2008).	1.40E-08
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
Log K_{ow} (unitless)	Hansch (1995).	2.61
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.	1.40E+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 organic carbon fraction of 0.01 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. 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)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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).	5.67E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-17

CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3.5E-02
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2.3E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1.3E-01
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2.3E-01
MCL	National Primary Drinking Water Regulations.	3.0E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Notes: NA = Not applicable
ND = No data available

TABLE A-1-18

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. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-18

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	HEAST (U.S. EPA 1997c).	5E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-19

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	Experimentally measured value (Allou et al. 2011).	3.1E-05
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
Log K_{ow} (unitless)	Hansch (1995).	1.48
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.	1.78E+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. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.78E-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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.33E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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).	7.80E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-19

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
Oral CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	4E-03
RfC (mg/m^3)	--	ND
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-20

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+03
H (atm·m^3/mol)	Experimentally measured value (Kim and Kim 2014).	5.9E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.80E-06
Log K_{ow} (unitless)	Hansch (1995).	2.13
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.60E-01
t (hr/event)*	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)	2.45E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4.0E-03

TABLE A-1-20

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	5.5E-02
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	3E-02
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2.8E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	4.6E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-21

CHEMICAL-SPECIFIC INPUTS FOR BENZIDINE (92-87-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	184.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.65
Vp (atm)	--	ND
S (g/2500ml)	Geometric mean value cited in U.S. EPA (1994c).	1.0
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Group Contribution Method described in Hine and Mookerjee (1975).	7.05E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.50E-05
Log K_{ow} (unitless)	Hansch (1995).	1.34
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.	2.08E+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.	2.08E-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.	1.56E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.60E-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)	6.14E+00

TABLE A-1-21

CHEMICAL-SPECIFIC INPUTS FOR BENZIDINE (92-87-5)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.3E+02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1.1E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.4E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.5E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-22

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)	Experimentally measured value (Lee et al. 2012).	5.90E-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
Log K_{ow} (unitless)	Wang (1986).	5.76
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.20E+00
t (hr/event)*	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
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 1993a).	1E-01
RfC (mg/m^3)	--	ND

TABLE A-1-22

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Inhalation CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(a)anthracene of 0.1 (U.S. EPA 1993a).	2E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	2.7E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-23

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.33E-03
H (atm·m^3/mol)	Experimentally measured value (ten Hulscher et al. 1992).	6.6E-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
Log K_{ow} (unitless)	Wang (1986).	5.78
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.	4.81E+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.	4.81E+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.	3.64E+04
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.40E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E+00
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-23

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

Parameter	Reference and Explanation	Value
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 1993a).	1E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Inhalation CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.1 (U.S. EPA 1993a).	2E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-24

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 25°C (solid)
S (mg/L)	U.S. EPA (1994b)	8.0E-04
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	9.43E-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
Log K_{ow} (unitless)	De Maagd (1998).	6.11
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.	1.01E+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.	1.04E+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.	7.61E+04
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.00E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.03E+00
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-24

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

Parameter	Reference and Explanation	Value
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 1993a)	1E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Inhalation CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.01 (U.S. EPA 1993a).	2E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-25

CHEMICAL-SPECIFIC INPUTS FOR BENZO(GHI)PERYLENE (191-24-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	276.34
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Experimentally measured value (ten Hulscher et al. 1992).	3.3E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	2.01E-02
D_w (cm^2/s)	D_W value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	5.26E-06
Log K_{ow} (unitless)	Hansch (1995).	6.63
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.	3.29E+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.	3.29E+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.	2.47E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.62E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.24E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.16E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW_{tissue})	--	ND

TABLE A-1-25

CHEMICAL-SPECIFIC INPUTS FOR BENZO(GHI)PERYLENE (191-24-2)

Parameter	Reference and Explanation	Value
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).	1.70E+06
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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-26

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.94E-03
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	1.58E-06
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
Log K_{ow} (unitless)	De Maagd (1998).	6.13
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04

TABLE A-1-26

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1E+00
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-06
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.4E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-27

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	Experimentally measured value (Li et al. 2007).	3.4E-08
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
Log K_{ow} (unitless)	Hansch (1995).	1.87
K_{oc} (mL/g)	U.S. EPA (1996a). The default value used by DRAS is based on the most neutral pH (6.8).	5.5 at pH=4.9 0.6 at pH=6.8 0.5 at pH=8.0
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. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.00E-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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.50E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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).	1.55E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E+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 72 kg.	1E+01

TABLE A-1-27

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-28

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	288.29
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-04 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	4.00E+04
H (atm·m^3/mol)	Experimentally measured value (Altschuh et al. 1999).	2.70E-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
Log K_{ow} (unitless)	Hansch (1995).	1.1
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.	8.90E+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.	8.90E-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.	6.68E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.60E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	1E-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 72 kg.	4E-01

TABLE A-1-28

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	3.75E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-29

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.90E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	5.035E-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
Log K_{ow} (unitless)	Hansch (1995).	2.3
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.	7.94E+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.	7.94E-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.	5.95E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E-01
t (hr/event)*	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)	3.30E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	2E-03
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.7E-01

TABLE A-1-29

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	1E-03
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.8E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-30

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	9.01
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,560
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.39E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.08E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	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
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	6.20E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-03
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-30

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	8.6E+00
MCL	National Primary Drinking Water Regulations.	4.00E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.10E+00

Notes: NA = Not applicable
ND = No data available

TABLE A-1-31

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-CHLOROETHOXY) METHANE (111-91-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1990)	173.04
T_m (°K)	Montgomery and Welkom (1990)	240.35
Vp (1mm @53 °C)	Montgomery and Welkom (1990)	1.0
S (mg/L@ 25 °C)	All metals, except mercury, are assumed to be insoluble in water.	81,000.00
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	3.85E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.20E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.46E-06
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	1.3
K_{oc} (mL/g)	Montgomery and Welkom (1990)	1.14E+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 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.	1.14E+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.	8.55E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	131E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.95E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.39E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.82E-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).	5.73

TABLE A-1-31

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-CHLOROETHOXY) METHANE (111-91-1)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	3E-03
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.	
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-32

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 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.70E+03
H (atm·m^3/mol)	Calculated value (Zhang et al. 2010).	3.0E-02
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
Log K_{ow} (unitless)	K_{ow} value cited in Howard (1989 - 1993).	2.58
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.	3.44E+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.	3.44E+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.	2.58E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.02E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.70E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	4E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND

TABLE A-1-32

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

Parameter	Reference and Explanation	Value
Inhalation [1] *CSF* (mg/kg/day)$^{-}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-33

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.18E+04
H (atm·m^3/mol)	Calculated value (Zhang et al. 2010).	2.1E-03
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
Log K_{ow} (unitless)	Hansch (1995).	1.29
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.50E-01
t (hr/event)*	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)	5.63E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.1E+00
RfC (mg/m^3)	--	ND

TABLE A-1-33

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.2E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.380E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-34

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.54
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	218.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	8.49E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1998c).	3.96E-01
H (atm·m^3/mol)	Calculated value (Cousins and MacKay 2000).	3.90E-05
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
Log K_{ow} (unitless)	DeBruijn (1989).	7.6
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.10E+01
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA

TABLE A-1-34

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

Parameter	Reference and Explanation	Value
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)	IRIS (U.S. EPA 2020b).	2E-02
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.4E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	7E-02
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	8.4E-03
MCL	National Primary Drinking Water Regulations.	6.0E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	3.2E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-35

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.97E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.907E-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
Log K_{ow} (unitless)	Sangster (1994).	2.0
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.	4.59E+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.	4.59E-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.	3.45E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.90E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.70E-01
t (hr/event)*	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)	1.95E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b)	2E-02
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b)	6.2E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	7E-02

TABLE A-1-35

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	6.2E-02
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	--	ND

Notes NA = Not applicable
ND = No data available

TABLE A-1-36

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.21E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	4.542E-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
Log K_{ow} (unitless)	Chem Inspect Test Inst. (1992).	2.4
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E+00
t (hr/event)*	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)	3.93E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-02
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	7.9E-03
RfC (mg/m^3)	--	ND

TABLE A-1-36

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	3.9E-03
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.93E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-37

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)	Experimentally measured value (Lau et al. 2006).	2.0E-04
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
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	4.94
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for most semivolatile nonionizing organic compounds cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.18E+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.	7.18E+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.	5.39E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	6.30E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.89E+00
t (hr/event)*	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* value was calculated by multiplying a food chain multiplier (*FCM*), 3.18, with an estimated *BCF*, 3.35E+03. *BCF*s were estimated using the correlation equation with K_{ow}obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995e).	1.06E+04
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-37

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

Parameter	Reference and Explanation	Value
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 (1996c)	1.5E+00

Notes: NA = Not applicable
ND = No data available

TABLE A-1-38

CHEMICAL-SPECIFIC INPUTS FOR BUTANOL (71-36-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	74.12
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	8.60E-03
S (mg/L)	U.S. EPA (1995g)	7.50E+04
H (atm·m^3/mol)	Experimentally measured value (Shunthirasingham et al. 2013).	9.9E-06
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	9.30E-06
Log K_{ow} (unitless)	Hansch (1995).	0.88
K_{oc} (mL/g)	U.S. EPA (1995g)	6.10E+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.	6.10E-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.	4.58E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.50E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.30E-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)	2.75E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-38

CHEMICAL-SPECIFIC INPUTS FOR BUTANOL (71-36-3)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-39

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.58E+00
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	9.53E-08
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
Log K_{ow} (unitless)	Ellington (1996).	4.73
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	7.00E+00
t (hr/event)*	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

TABLE A-1-39

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

Parameter	Reference and Explanation	Value
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)	5.68E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-01
Oral CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	1.9E-03
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	7E-01
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.9E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.9E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-40

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-4,6-DINITROPHENOL, 2-SEC (DINOSEB) (88-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	240.22
T_m (K)	U.S. EPA (1995b)	311.15 to 414.15
Vp (atm)	U.S. EPA (1995g)	9.90E-05
S (mg/L)	U.S. EPA (1995g)	5.20E+01
H (atm·m^3/mol)	Experimentally measured value (Tremp et al. 1993).	4.5E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	3.56
K_{oc} (mL/g)	U.S. EPA (1995g)	1.20E+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.	1.20E+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.	9.00E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.60E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.30E+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)	2.96E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-40

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-4,6-DINITROPHENOL, 2-SEC (DINOSEB) (88-85-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-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 72 kg.	4E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7.0E-03
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-41

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.41
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	594.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.16E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.45E-06
Log 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. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	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
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	9.07E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-41

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	ATSDR MRL (ATSDR 2020).	1E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	6.5E+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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-42

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.67E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.722E-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
Log K_{ow} (unitless)	Hansch (1995).	1.94
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.	4.12E+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.	4.12E-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.	3.09E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	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)	1.76E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-42

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	7E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	1E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-43

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.92E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.986E-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
Log K_{ow} (unitless)	Hansch (1995).	2.83
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	7.60E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-03
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	7E-02
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-01

TABLE A-1-43

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.2E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.52E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-44

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.51E-01
H (atm·m^3/mol)	Experimentally measured value (Fendinger et al. 1989).	5.5E-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
Log K_{ow} (unitless)	Simpson (1995).	6.16
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.80E+01
t (hr/event)*	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)	--	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)	5.63E+05
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04

TABLE A-1-44

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	3.5E-01
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	7E-04
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	3.6E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-45

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.90
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	172.1
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	--	1.10E-01
D_w (cm^2/s)	--	1.27E-05
Log 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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	CalEPA (2020)	2E-04
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	4E+00 MRDL

TABLE A-1-45

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

Parameter	Reference and Explanation	Value
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-46

CHEMICAL-SPECIFIC INPUTS FOR CHLOROANILINE, p- (106-47-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Group Contribution Method described in Hine and Mookerjee (1975).	1.86E-06
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
Log K_{ow} (unitless)	Hansch (1995).	1.83
K_{oc} (mL/g)	--	6.00E-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. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.00E-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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.50E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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)	1.45E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-03

TABLE A-1-46

CHEMICAL-SPECIFIC INPUTS FOR CHLOROANILINE, p- (106-47-8)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	2E-01
RfC (mg/m^3)	--	ND
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-47

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.09E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.676E-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
Log K_{ow} (unitless)	Sangster (1994).	2.84
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.30E-01
t (hr/event)*	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)	8.48E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	5E-02

TABLE A-1-47

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

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-48

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 25°C (solid)
S (mg/L)	Howard (1989-1993)	1.30E+01
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	1.30E-07
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
Log K_{ow} (unitless)	Chem Inspect Test Inst (1992).	4.74
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.	4.57E+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. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.57E+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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.43E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.50E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.40E+00
t (hr/event)*	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)	5.78E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-02
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	1.1E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	7E-02

TABLE A-1-48

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.1E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORO-1,3-BUTADIENE (CHLOROPRENE) (126-99-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	88.54
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	2.80E-01
S (mg/L)	U.S. EPA (1995g)	6.30E+02
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	5.61E-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)	1.00E-05
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	2.53
K_{oc} (mL/g)	U.S. EPA (1995g)	1.10E+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. 5g)	1.10E+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.	8.25E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.30E-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).	4.93E+01

TABLE A-1-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORO-1,3-BUTADIENE (CHLOROPRENE) (126-99-8)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	2E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-50

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 25ºC (liquid)
S (mg/L)	Howard 1989-1993	2.90E+03
H (atm·m^3/mol)	Experimentally measured value (Zheng et al. 1997).	2.7E-02
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
Log K_{ow} (unitless)	Hansch (1995).	1.08
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.	8.58E+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.	8.58E-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.	6.44E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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)	3.90E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmark		
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E+01
Oral CSF (mg/kg/day)$^{-1}$		ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5+01

TABLE A-1-50

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$		ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-51

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 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994a)	5.74E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.152E-02
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
Log K_{ow} (unitless)	Hansch (1995).	1.43
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.	1.62E+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.	1.62E-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.	1.22E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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)	7.19E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	Subchronic PPRTV (U.S. EPA 2020c).	1E-01

TABLE A-1-51

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$		ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E+01
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-52

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.96E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	3.571E-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
Log K_{ow} (unitless)	Hansch (1995).	1.97
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.70E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)		1E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-52

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	ATSDR MRL (ATSDR 2020).	9.8E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	8.3E-02
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.89+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-53

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)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	2.45E-06
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
Log K_{ow} (unitless)	Hansch (1995).	3.1
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.	3.41E+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.	3.41E+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.	2.56E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	4.09E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.50E-01
t (hr/event)*	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

TABLE A-1-53

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

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	ATSDR MRL (ATSDR 2020). Value used is for cresols and is same value used for RSLs.	1E-01
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-54

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

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.36E+03
H (atm·m^3/mol)	Experimentally measured value (Shiu and Mackay 1997).	3.30E-04
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
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	3.9
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E-01
t (hr/event)*	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).	5.42E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-54

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-02
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-55

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)	Experimentally measured value (Sheikheldin et al. 2001).	6.51E-06
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
Log K_{ow} (unitless)	Hansch (1995).	2.15
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.30E-01
t (hr/event)*	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
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)	2.54E+01

TABLE A-1-55

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

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-03
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 (1996c)	4.4E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-56

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 25°C (liquid)
S (mg/L)	*S* value cited in Montgomery and Welkom (1991).	3.30E+00
H (atm·m^3/mol)	Calculated value (Hilal et al. 2008).	3.2E-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
Log K_{ow} (unitless)	Kurz (1999).	4.7
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.	6.31E+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.	6.31E+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.	4.74E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		

TABLE A-1-56

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

Parameter	Reference and Explanation	Value
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)	4.78E+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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-57

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (+3) (16065-38-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	51.996
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2173.15
Vp (atm)	--	0
S (mg/L)	--	0
H (atm·m^3/mol)	--	0
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.01E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.63E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/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. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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 (1998b).	1.90E+01
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		

TABLE A-1-57

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (+3) (16065-38-1)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1.5E+00
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.	1.0E-01
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-58

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.0
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.58E-05
Log 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. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.90E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-03
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	5.0E-01

TABLE A-1-58

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-04
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b) for Chromium (+6) adjusted for the proportion of Cr(+6) in the original study (1 part in 7).	2.9E+02
MCL	National Primary Drinking Water Regulations.	1.0E-01
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.10E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-59

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.94E-03
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	4.70E-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
Log K_{ow} (unitless)	De Maagd (1998).	5.81
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.	5.15E+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.	5.15E+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.	3.86E+04
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	8.60E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.20E+00
t (hr/event)*	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

TABLE A-1-59

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

Parameter	Reference and Explanation	Value
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 1993a)	1E-03
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the Inhalation CSF for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.1 (U.S. EPA 1993a).	2E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-60

CHEMICAL-SPECIFIC INPUTS FOR CIS-1,3-DICHLOROPROPENE (10061-01-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.97
T_m (°K)	--	
Vp (atm)	U.S. EPA (1995g)	4.99E-02
S (mg/L)	U.S. EPA (1995g)	2.70E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.031E-03
D_a (cm^2/s)	U.S. EPA (1995g)	5.85E-02
D_w (cm^2/s)	U.S. EPA (1995g)	1.10E-05
Log K_{ow} (unitless)	Tomlin (1997)	2.06
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+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.	9.30E-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.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	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)	*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)	2.17E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-60

CHEMICAL-SPECIFIC INPUTS FOR CIS-1,3-DICHLOROPROPENE (10061-01-5)

Parameter	Reference and Explanation	Value
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 (µg/l)	U.S. EPA (1995f)	2.40E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-61

CHEMICAL-SPECIFIC INPUTS FOR COBALT (7440-48-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	58.93
T_m (K)	Montgomery and Welkom (1991)	1766.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	3E-4
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	6E-06
Inhalation CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	3E+01
MCL	National Primary Drinking Water Regulations.	ND

TABLE A-1-61

CHEMICAL-SPECIFIC INPUTS FOR COBALT (7440-48-4)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-62

CHEMICAL-SPECIFIC INPUTS FOR COPPER (7440-50-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	63.55
T_m (K)	Montgomery and Welkom (1991)	1356.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	2.20E+01
Kd_{sw} (L/Kg)	--	2.20E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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 (1998b).	7.10E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	ATSDR intermediate MRL (ATSDR 2020).	1E-02
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.	1.3

TABLE A-1-62

CHEMICAL-SPECIFIC INPUTS FOR COPPER (7440-50-8)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	9.00E+00

Notes: NA = Not applicable
ND = No data available

TABLE A-1-63

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)	Experimentally measured value (Feigenbrugel et al. 2004b).	1.2E-06
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
Log K_{ow} (unitless)	Hansch (1995).	1.96
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.	8.45E+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.	8.45E-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.	6.34E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	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)	1.82E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	CalEPA (2020) value for mixed cresols.	6E-01
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-63

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

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-64

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)	Experimentally measured value (Feigenbrugel et al. 2004b).	2.3E-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
Log K_{ow} (unitless)	Hansch (1995).	1.95
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.	8.26E+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.	8.26E-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.	6.20E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	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)	1.79E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	CalEPA (2020) value for mixed cresols.	6E-01
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-64

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

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-65

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)	Experimentally measured value (Feigenbrugel et al. 2004b).	9.9E-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
Log K_{ow} (unitless)	Hansch (1995).	1.94
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.	8.08E+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.	8.08E-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.	6.20E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.00E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	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)	1.76E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	ATSDR MRL (ATSDR 2020).	1E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-65

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	CalEPA (2020) value for mixed cresols.	6E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-66

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)	Experimentally measured value (Hiatt 2013).	7.070E-03
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
Log K_{ow} (unitless)	Hansch (1995).	3.66
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.	9.48E+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. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.48E+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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.11E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.20E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.70E-01
t (hr/event)*	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)	3.56E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
Oral CSF (mg/kg/day)$^{-1}$	--	NA
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	4E-01
Inhalation CSF (mg/kg/day)$^{-1}$	--	NA

TABLE A-1-66

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

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-67
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 25°C (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
Log K_{ow} (unitless)	Hansch (1995).	-0.25
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	U.S. EPA (1996a).	9.9
Kd_{sw} (L/Kg)	U.S. EPA (1996a).	9.9
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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)	IRIS (U.S. EPA 2020b).	6.3E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2010)	8E-04
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-1-67
CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

Notes: NA = Not applicable
ND = No data available

TABLE A-1-68

CHEMICAL-SPECIFIC INPUTS FOR CYCLOTETRAMETHYLENETETRANITRAMINE (HMX) (2691-41-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	296.16
T_m (K)	CRC Handbook (1995)	559.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	8.67E-10
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-06
Log K_{ow} (unitless)	Monteil-Rivera (2003).	0.16
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.28E-05
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	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 72 kg.	1.75E-01
	--	ND

TABLE A-1-68

CHEMICAL-SPECIFIC INPUTS FOR CYCLOTETRAMETHYLENETETRANITRAMINE (HMX) (2691-41-0)

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$		
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-69

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)	Experimentally measured value (Cetin et al. 2006).	1.1E-05
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
Log K_{ow} (unitless)	Sangster (1994).	6.02
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	7.80E+00
t (hr/event)*	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)	3.94E+05
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	3E-05
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 20204b).	2.4E-01

TABLE A-1-69

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E-04
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.4E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	6.4E-03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-70

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.92E-02
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	6.2E-05
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
Log K_{ow} (unitless)	Sangster (1993).	6.51
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	7.60E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	3E-04
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 20204b).	3.4E-01

TABLE A-1-70

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

Parameter	Reference and Explanation	Value
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)	1.05E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-71

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.41E-03
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	1.1E-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
Log K_{ow} (unitless)	Hansch (1995).	6.91
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.30E+01
t (hr/event)*	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)	2.76E+06
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	5E-04
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 20204b).	3.4E-01

TABLE A-1-71

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	2E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	3.50E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-72

CHEMICAL-SPECIFIC INPUTS FOR DIALLATE (2303-16-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	270.24
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.00E-07
S (ppm)	*S* value cited in U.S. EPA (1995b).	40
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	7.87E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Ellington (1988).	4.49
K_{oc} (mL/g)	Value cited in U.S. EPA (1995g).	2.60E+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.	2.60E+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.	1.82E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.60E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.10E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-72

CHEMICAL-SPECIFIC INPUTS FOR DIALLATE (2303-16-4)

Parameter	Reference and Explanation	Value
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)	2.69E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	HEAST (U.S. EPA 1997c).	6.1E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	6.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-73

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

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)	Experimentally measured value (Feigenbrugel 2004a).	6.6E-07
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
Log K_{ow} (unitless)	Hansch (1995).	3.81
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.	5.57E+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 organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.57E+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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.17E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.10E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.40E+00
t (hr/event)*	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)	*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)	463.02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	ATSDR MRL (ATSDR 2020).	7.0E-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 72 kg.	2.5E-03

TABLE A-1-73

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-74

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)	Calculated value (Hilal et al. 2008).	8.20E-07
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
Log K_{ow} (unitless)	Sangster (1993).	6.75
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.40E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	--	ND

TABLE A-1-74

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

Parameter	Reference and Explanation	Value
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 1993b).	1E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Calculated by multiplying the Inhalation CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 1.0 (U.S. EPA 1993b).	2E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-75

CHEMICAL-SPECIFIC INPUTS FOR DIBENZOFURAN (132-64-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	168.19
T_m (K)	CRC Handbook (1995)	359.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	2.13E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	4.12
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.06E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	2.04E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	1E-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 72 kg.	4E-03
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-75

CHEMICAL-SPECIFIC INPUTS FOR DIBENZOFURAN (132-64-9)

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	2.00E+1

Notes: NA = Not applicable
ND = No data available

TABLE A-1-76

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.44E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	9.215E-04
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
Log K_{ow} (unitless)	Sangster (1994).	2.16
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.	6.15E+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.	6.15E-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.	4.61E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.50E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.60E+00
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-76

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

Parameter	Reference and Explanation	Value
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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	2E-02
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	8.4E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	7.2E-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.	8.0E-02 TTHM
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-77

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.20E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.013E-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
Log K_{ow} (unitless)	Chemical Inspect Test Inst. (1992).	2.96
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.	2.64E+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 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.	2.64E+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.	1.98E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.40E+00
t (hr/event)*	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)	1.05E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	2E-04
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	8E-01

TABLE A-1-77

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	2E-04
Inhalation CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	2E+01
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-78

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.25E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.231E-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
Log K_{ow} (unitless)	Hansch (1995).	3.43
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	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)	2.38E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-78

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	9E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	HEAST (U.S. EPA 1997c).	2E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	6.0E-01
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.4E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-79

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)	Experimentally measured value (Hiatt 2013).	1.877E-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
Log K_{ow} (unitless)	Hansch (1995).	3.53
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.	7.48E+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.	7.48E+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.	5.61E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	8.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-79

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

Parameter	Reference and Explanation	Value
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 (1996c)	7.1E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-80

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+01
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.697E-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
Log K_{ow} (unitless)	Hansch (1995).	3.44
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	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)	2.42E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-80

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	ATSDR MRL (ATSDR 2020).	7E-02
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	5.4E-03
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	8E-01
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	4E-02
MCL	National Primary Drinking Water Regulations.	7.5E-02
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.5E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-81

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.52E+00
H (atm·m^3/mol)	Calculated value (Mackay et al. 2006).	4.9E-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
Log K_{ow} (unitless)	Hansch (1995).	3.51
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.	7.21E+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.	7.21E+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.	5.41E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.10E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	--	NA
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 20204b).	4.5E-01

TABLE A-1-81

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

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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-82

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.0E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	7.833E-02
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
Log K_{ow} (unitless)	Hansch (1995).	2.16
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.	6.15E+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.	6.15E-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.	4.61E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.20E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.80E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	2E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-82

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Screening PPRTV (U.S. EPA 2020c).	1E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-83

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.16E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	4.972E-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
Log K_{ow} (unitless)	Hansch (1995).	1.79
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.50E-01
t (hr/event)*	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)	1.35E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-83

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	2E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	HEAST (U.S. EPA 1997c).	5E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.58E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-84

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.31E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.204E-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
Log K_{ow} (unitless)	Hansch (1995).	1.48
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.50E-01
t (hr/event)*	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)	7.85E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-84

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	6E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	9.1E-02
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	7E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	9.4E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.0E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-85

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.0E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.419E-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
Log K_{ow} (unitless)	Hansch (1995).	2.13
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.40E-01
t (hr/event)*	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)	2.48E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-85

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	5E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	2E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.03E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-86

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.94E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	3.666E-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
Log K_{ow} (unitless)	Hansch (1995).	1.86
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.	3.56E+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.	3.56E-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.	2.67E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.40E-01
t (hr/event)*	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)	1.53E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	2E-03

TABLE A-1-86

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

Parameter	Reference and Explanation	Value
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.	7E-02
Aquatic TRV (ug/l)	Suter (1996)	5.72E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-87

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	6.03E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	9.647E-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
Log K_{ow} (unitless)	Hansch (1995).	2.09
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.40E-01
t (hr/event)*	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)	2.28E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-87

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	2E-02
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.	1E-01
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.4E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-88

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)	Experimentally measured value (Sheikheldin et al. 2001).	2.90E-06
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
Log K_{ow} (unitless)	Hansch (1995).	3.06
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.60E-01
t (hr/event)*	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
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+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-88

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	3E-03
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)	3.6E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-89

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DICHLOROPHENOL (87-65-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	163.01
T_m (K)	Howard (1989-1993)	337.65 to 338.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Calculated value (Mackay et al. 2006).	7.6E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
Log K_{ow} (unitless)	Hansch (1995).	2.75
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.07E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.63E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.07E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.24E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
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

TABLE A-1-89

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DICHLOROPHENOL (87-65-0)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOXYACETIC ACID (94-75-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	221.04
T_m (K)	--	ND
Vp (atm)	U.S. EPA (1995g)	1.40E-05
S (mg/L)	U.S. EPA (1995g)	6.80E+02
H (atm·m^3/mol)	Calculated value (Suntio et al. 1988).	5.5E-06
D_a (cm^2/s)	U.S. EPA (1995g)	5.88E-02
D_w (cm^2/s)	U.S. EPA (1995g)	6.49E-06
Log K_{ow} (unitless)	Hansch (1995).	2.81
K_{oc} (mL/g)	U.S. EPA (1995g)	4.50E+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 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.--	4.50E+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.	3.37E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.10E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.70E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.00E-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)	8.05E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOXYACETIC ACID (94-75-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	1E-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 72 kg.	4E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7.0E-02
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-91

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.68E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.303E-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
Log K_{ow} (unitless)	Sangster (1994).	1.98
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.30E-01
t (hr/event)*	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
Health Benchmarks		

TABLE A-1-91

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

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	4E-02
Oral CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	3.7E-02
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	4E-03
Inhalation CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	1.3E-02
MCL	National Primary Drinking Water Regulations.	5.0E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.25E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-92

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)	Experimentally measured value (Wright et al. 1992).	1.5E-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
Log K_{ow} (unitless)	Tomlin (1997).	2.03
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	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)	2.05E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-92

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	3E-02
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	1E-01
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	2E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	4.00E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-93

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE-TRANS (10061-02-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.695E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	Tomlin (1997).	2.03
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+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 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.	9.30E-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.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	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)	2.05E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-93

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE-TRANS (10061-02-6)

Parameter	Reference and Explanation	Value
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 (µg/l)	U.S. EPA (1995f)	2.40E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-94

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	Experimentally measured value (Gautier et al. 2003).	2.5E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	1.43
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+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 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.	9.30E-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.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	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).	7.19E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-94

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.9E-01
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5E-04
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.9E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-95

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 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a)	1.87E-01
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	1.1E-05
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
Log K_{ow} (unitless)	DeBruijn (1989).	5.4
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.80E+01
t (hr/event)*	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)	4.36E+04
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-05
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.6E+01

TABLE A-1-95

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	2E-04
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.7E+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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-96

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.80E+02
H (atm·m^3/mol)	Calculated value (Sacan et al. 2005).	1.7E-06
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
Log K_{ow} (unitless)	Ellington (1996).	2.42
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.00E+00
t (hr/event)*	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)	*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)	4.07E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-96

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-01
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 (1996c)	2.2E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-97

CHEMICAL-SPECIFIC INPUTS FOR DIETHYLSTILBESTROL (56-53-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	443.65
Vp (atm)	U.S. EPA (1995g)	1.40E-12
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.30E+04
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribuition Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	5.80E-12
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	5.07
K_{oc} (mL/g)	U.S. EPA (1995g)	9.60E+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.	9.60E+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.	7.20E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+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

TABLE A-1-97

CHEMICAL-SPECIFIC INPUTS FOR DIETHYLSTILBESTROL (56-53-1)

Parameter	Reference and Explanation	Value
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)	6.80E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	3.5E+02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	3.5E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-98

CHEMICAL-SPECIFIC INPUTS FOR DIMETHOATE (60-51-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	Calculated value (Mackay et al. 2006).	1.1E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	Hansch (1995).	0.78
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+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 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.	9.30E-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.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	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)	2.31E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-98

CHEMICAL-SPECIFIC INPUTS FOR DIMETHOATE (60-51-5)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	OPP HHBP (U.S. EPA 2020d).	2.2E-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 72 kg.	7.9E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-99

CHEMICAL-SPECIFIC INPUTS FOR 7,12-DIMETHYLBENZ(A)ANTHRACENE (57-97-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	256.35
T_m (K)	--	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.80E-12
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.00E-02
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribuition Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	6.10E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.98E-06
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	5.8
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for most semivolatile nonionizing organic compounds cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.03E+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 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.	5.03E+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.	3.77E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.60E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.20E+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* value was calculated by multiplying a food chain multiplier (*FCM*), 12.1, with an estimated *BCF*, 1.51E+04. *BCF*s were estimated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995e).	1.82E+05
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2.5E+02

TABLE A-1-99

CHEMICAL-SPECIFIC INPUTS FOR 7,12-DIMETHYLBENZ(A)ANTHRACENE (57-97-6)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.5E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-100

CHEMICAL-SPECIFIC INPUTS FOR 3-3'-DIMETHYLBENZIDINE (119-93-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	212.28
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.90E-10
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+03
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Group Contribution Method described in Hine and Mookerjee (1975).	8.10E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.83E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.17E-06
Log K_{ow} (unitless)	Hansch (1995).	2.34
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.	2.00E+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.	2.00E+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.	1.50E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.70E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.70E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.80E-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)	3.54E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	1.1E+01

TABLE A-1-100

CHEMICAL-SPECIFIC INPUTS FOR 3-3'-DIMETHYLBENZIDINE (119-93-7)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.1E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-101

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.19E+03
H (atm·m^3/mol)	Calculated value (Sacan et al. 2005).	1.0E-06
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
Log K_{ow} (unitless)	Ellington (1996).	1.6
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.	3.74E+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.	3.74E-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.	2.81E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.60E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.30E+00
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-101

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

Parameter	Reference and Explanation	Value
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
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)	U.S. EPA (1995f)	3.30E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-102

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)	Experimentally measured value (Sheikheldin et al. 2001).	1.50E-06
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
Log K_{ow} (unitless)	Hansch (1995).	2.3
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.90E-01
t (hr/event)*	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
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)	3.30E+01

TABLE A-1-102

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

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-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 72 kg.	7E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-103

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 25°C (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
Log K_{ow} (unitless)	Debnath (1992).	1.81
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.	6.02E+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.	6.02E-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.	4.51E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.70E+00
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-103

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

Parameter	Reference and Explanation	Value
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 $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	1.6E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-104

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.08E+01
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	1.06E-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
Log K_{ow} (unitless)	Ellington (1996).	4.5
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.40E+00
t (hr/event)*	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

TABLE A-1-104

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

Parameter	Reference and Explanation	Value
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)	2.74E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
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 (1996c)	3.0E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-105

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	5.4E+02
H (atm·m^3/mol)	Experimentally measured value (Altschuh et al. 1999).	4.9E-08
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
Log K_{ow} (unitless)	Hansch (1995).	1.49
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.	2.92E+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.	2.92E-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.	2.19E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.10E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.30E-01
*t** (hr/event)	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
Biotransfer Factors for Animals		

TABLE A-1-105

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

Parameter	Reference and Explanation	Value
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)	IRIS (U.S. EPA 2020b).	1E-04
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-106

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITRO-6-METHYLPHENOL (534-52-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	198.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	360.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Experimentally measured value (Tremp et al. 1993).	2.3E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.91E-06
Log K_{ow} (unitless)	Hansch (1995).	2.13
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.78E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.41E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.39E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.32E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	8E-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 72 kg.	3E-04
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND

TABLE A-1-106

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITRO-6-METHYLPHENOL (534-52-1)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-107

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.8E+03
H (atm·m^3/mol)	Experimentally measured value (Tremp et al. 1993).	9.0E-08
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
Log K_{ow} (unitless)	Hansch (1995).	1.67
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	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)	1.09E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-03
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND

TABLE A-1-107

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

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-108

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)	Experimentally measured value (Altschuh et al. 1999).	5.4E-08
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
Log K_{ow} (unitless)	Hansch (1995).	1.98
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.	8.84E+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.	8.84E-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.	6.63E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.90E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-03
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	3E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	3E-01

TABLE A-1-108

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

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.10E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-109

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)	Calculated value (Zhang et al. 2010).	2.3E-06
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
Log K_{ow} (unitless)	Nakagawa (1992).	2.1
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.	1.16E+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 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.	1.16E+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.	8.70E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.10E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	3E-04
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	1.5E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-109

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

Parameter	Reference and Explanation	Value
MCL	--	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.1E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-110

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+00
H (atm·m^3/mol)	Calculated value (Staples et al. 1997).	1.03E-04
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
Log K_{ow} (unitless)	Ellington (1996).	8.1
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.	9.17E+07
Kd_s (cm^3/g)	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.	9.17E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.88E+06
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	4.20E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.10E+01
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-110

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

Parameter	Reference and Explanation	Value
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)	PPRTV (U.S. EPA 2020c).	1E-02
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)	Suter (1996)	1.99E+03

Notes: NA = Not applicable
ND = No data availablee

TABLE A-1-111

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	9.00E+05
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	4.252E-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
Log K_{ow} (unitless)	Hansch (1995).	-0.27
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.	7.32E-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.	7.32E-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.	5.49E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.90E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	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)	3.67E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	3E-02
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1E-01

TABLE A-1-111

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	3E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	2E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-112

CHEMICAL-SPECIFIC INPUTS FOR DIPHENYLAMINE (122-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	169.23
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.60E-06
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+02
H (atm·m^3/mol)	Calculated value (Hilal et al. 2008).	3.3E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.31E-06
Log K_{ow} (unitless)	Hansch (1995).	3.5
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.	2.76E+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.	2.76E+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.	2.07E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	5.20E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.40E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-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)	2.69E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	OPP HHBP (U.S. EPA 2020d).	1E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-112

CHEMICAL-SPECIFIC INPUTS FOR DIPHENYLAMINE (122-39-4)

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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-113

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)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	4.78E-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
Log K_{ow} (unitless)	Hansch (1995).	2.94
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.	2.77E+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.	2.77E+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.	5.83E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	8E-01

TABLE A-1-113

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	7.9E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.7E+00

Notes: NA = Not applicable
ND = No data available

TABLE A-1-114

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 25°C (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
Log K_{ow} (unitless)	Hansch (1995).	4.02
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.	8.95E+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.	8.95E+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.	6.71E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.10E+00
t (hr/event)*	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)	--	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)	8.79E+02
Health Benchmarks		

TABLE A-1-114

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

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-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 72 kg.	1E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-115

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)	Calculated value (Mackay et al. 2006).	1.0E-05
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
Log K_{ow} (unitless)	Hansch (1995).	3.83
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.70E+01
t (hr/event)*	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)	4.80E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-115

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-03
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)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.6E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-116

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 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a)	2.46E-01
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	5.5E-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
Log K_{ow} (unitless)	DeBruijn (1989).	5.2
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.80E+01
t (hr/event)*	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)	2.01E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-116

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-117

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.60E+04
H (atm·m^3/mol)	Calculated value (Hilal et al. 2008).	1.04E-04
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
Log K_{ow} (unitless)	DeNeer (1988).	0.45
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.	2.72E+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.	2.72E-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.	2.04E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.80E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.20E-01
t (hr/event)*	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)	1.29E-00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	6E-03

TABLE A-1-117

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	9.9E-03
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-03
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	4.3E-03
MCL	National Primary Drinking Water Regulations.	2.0E+01 TT[7]
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-118

CHEMICAL-SPECIFIC INPUTS FOR 2-ETHOXYETHANOL (110-80-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	90.12
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.00E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+01
H (atm·m^3/mol)	Experimentally measured value (Johanson and Dynesius 1988).	1.1E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.57E-06
Log K_{ow} (unitless)	Hansch (1995).	-0.32
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.	6.68E-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.	6.68E-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.	5.01E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.60E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-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)	3.36E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	9E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-118

CHEMICAL-SPECIFIC INPUTS FOR 2-ETHOXYETHANOL (110-80-5)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-119

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ACETATE (141-78-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	88.1
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.20E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.40E+04
H (atm·m^3/mol)	Experimentally measured value (Fenclova et al. 2014).	1.6E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.66E-06
Log K_{ow} (unitless)	Hansch (1995).	0.73
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+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.	4.53E-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.	3.40E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	4.90E-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)	2.11E-00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	9E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-119

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ACETATE (141-78-6)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	7E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-120
CHEMICAL-SPECIFIC INPUTS FOR ETHYL ETHER (60-29-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.12
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.10E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.10E+04
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	8.680E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.40E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Hansch (1989).	0.89
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.	6.07E+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.	6.07E-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.	4.55E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.60E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-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)	2.80E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-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 72 kg.	7.2E-01

TABLE A-1-120
CHEMICAL-SPECIFIC INPUTS FOR ETHYL ETHER (60-29-7)

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-121

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 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.90E+04
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility per Meylan and Howard (1991).	5.73E-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
Log K_{ow} (unitless)	Hansch (1995).	1.94
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.	4.12E+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.	4.12E-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.	3.09E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.30E-01
t (hr/event)*	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)	1.76E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	9E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-121

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	3E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-122

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 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.90E+05
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	5.35E-06
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
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	-0.17
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for most semivolatile nonionizing organic compounds cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.81E-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.	6.81E-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.	5.11E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.60E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.00E-01
t (hr/event)*	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-1-122

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).	4.37E-01
BAF_{fish} (L/kg FW)	--	NA
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-123

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.73E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	4.855E-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
Log K_{ow} (unitless)	Hansch (1995).	3.15
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	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)	1.46E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-123

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.1E-02
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E+00
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	8.7E-03
MCL	National Primary Drinking Water Regulations.	7E-01
Aquatic TRV (ug/l)	U.S. EPA (1995f)	4.53E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-124

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.20E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	5.698E-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
Log K_{ow} (unitless)	Hansch (1995).	1.96
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.	4.27E+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.	4.27E-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.	3.20E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.40E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	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)	1.82E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 20204b).	9E-03
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 20204b).	2E+00

TABLE A-1-124

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	9E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 20204b).	2E+00
MCL	National Primary Drinking Water Regulations.	5E-05
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-125

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE THIOUREA (ETU) (96-45-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	102.17
T_m (°K)	Budavari, O'Neill, Smith, and Heckelman (1989)	476.65
Vp	Geometric mean value cited in U.S. EPA (1994c).	1.10E-04
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+04
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	3.36E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
Log K_{ow} (unitless)	Govers (1986).	-0.66
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.	2.25E-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.	2.25E-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.	1.68E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-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)	1.86E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-05

TABLE A-1-125

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE THIOUREA (ETU) (96-45-7)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	4.5E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	3E-04
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	4.5E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-126

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)	Experimentally measured value (Lee et al. 2012).	2.93E-05
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
Log K_{ow} (unitless)	Hansch (1995).	5.16
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.50E+00
t (hr/event)*	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

TABLE A-1-126

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

Parameter	Reference and Explanation	Value
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)	2.06E+04
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-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 72 kg.	1E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-127

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	166.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	389.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	8.17E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	1.90E+00
H (atm·m^3/mol)	Experimentally measured value (Lee et al. 2012).	3.07E-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
Log K_{ow} (unitless)	Hansch (1995)	4.18
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.00E-01
t (hr/event)*	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)	1.22E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-127

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-128

CHEMICAL-SPECIFIC INPUTS FOR FLUORIDE (16984-48-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	18.9984
T_m (K)	--	NA
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a was calculated using equations cited and recommended for use in U.S. EPA (1997g).	0.26684
D_w (cm^2/s)	D_w was calculated using equations cited and recommended for use in U.S. EPA (1997g).	3.09E-05
Log K_{ow} (unitless)	U.S. EPA (2000).	2.23E-01
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	--	NA
τ (hr)	--	NA
t (hr/event)*	--	NA
B	--	NA
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	CalEPA (2020)	4E-02
Oral CSF (mg/kg/day)$^{-1}$	--	NA
RfC (mg/m^3)	CalEPA (2020)	1.3E-02
Inhalation CSF (mg/kg/day)$^{-1}$	--	NA

TABLE A-1-128

CHEMICAL-SPECIFIC INPUTS FOR FLUORIDE (16984-48-8)

Parameter	Reference and Explanation	Value
MCL (mg/L)	National Primary Drinking Water Regulations.	4
Aquatic TRV (µg/l)	--	NA

Notes: NA = Not applicable
ND = No data available

TABLE A-1-129

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	30.03
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	365.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c)	5.10E+00 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	5.50E+05
H (atm·m^3/mol)	Experimentally measured value (Liu et al. 2015).	2.8E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.80E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.98E-05
Log K_{ow} (unitless)	Hansch (1995).	0.35
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.	2.27E+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.	2.27E-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.	1.70E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.30E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-01

TABLE A-1-129

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2.1E-02
RfC (mg/m^3)	ATSDR MRL (ATSDR 2020).	9.8E-03
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	4.7E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-130

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	46.03
T_m (K)	U.S. EPA (1995g)	282.0
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	5.40E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	1.00E+06
H (atm·m^3/mol)	Experimentally measured value (Johnson et al. 1996).	1.10E-07
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
Log K_{ow} (unitless)	Hansch (1995)	-0.54
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.	4.47E-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 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.	4.47E-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.	3.36E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	4.10E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.70E-01
t (hr/event)*	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)	2.29E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	9E-01

TABLE A-1-130

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	Screening PPRTV (U.S. EPA 2020c).	3.E-04
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-131

CHEMICAL-SPECIFIC INPUTS FOR FURAN (110-00-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	68.08
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.90E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+04
H (atm·m^3/mol)	Calculated value (Mackay et al. 2006).	5.40E-03
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).	1.22E-05
Log K_{ow} (unitless)	Hansch (1995).	1.34
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.	1.38E+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 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.	1.38E-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.	1.03E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.50E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-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)	6.14E+00

TABLE A-1-131

CHEMICAL-SPECIFIC INPUTS FOR FURAN (110-00-9)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1-03
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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-132

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)	Experimentally measured value (Cetin et al. 2006).	5.2E-04
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
Log K_{ow} (unitless)	Simpson (1995).	6.1
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.70E+01
t (hr/event)*	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 $_{FW\ tissue}$)	*BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	5.52E+03

TABLE A-1-132

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

Parameter	Reference and Explanation	Value
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 *BCF*. *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998).	1.05E+05
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	4.5E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	4.7E+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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-133

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	389.32
T_m (K)	Montgomery and Welkom (1991)	430.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	5.79E-09 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a) .	2.68E-01
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	2.0E-05
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
Log K_{ow} (unitless)	Sangster (1993).	4.98
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.	7.86E+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.	7.86E+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.	5.90E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.90E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.10E+01
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-133

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

Parameter	Reference and Explanation	Value
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)	1.14E+04
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1.3E-05
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	9.1+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	4.7E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	9.4E+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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-134

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)	Experimentally measured value (Hiatt 2013).	4.187E-03
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
Log K_{ow} (unitless)	Hansch (1995).	4.78
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.	5.00E+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.	5.00E+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.	3.75E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.30E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.40E+00
t (hr/event)*	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)	6.20E+03
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	1E-03
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	7.8E-02
RfC (mg/m^3)	--	ND

TABLE A-1-134

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

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	7.9E-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-1-135

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	8.62E-03
H (atm·m^3/mol)	Experimentally measured value (McPhedran et al. 2013).	3.0E-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
Log K_{ow} (unitless)	DeBruijn (1989).	5.73
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.80E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-04

TABLE A-1-135

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.6E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.7E+00
MCL	National Primary Drinking Water Regulations.	1E-03
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-136

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, ALPHA (ALPHA-BHC) (319-84-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	3.3E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.8
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+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.	4.60E+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.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-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)	4.56E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-136

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, ALPHA (ALPHA-BHC) (319-84-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	ATSDR MRL (ATSDR 2020).	8.0E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	6.3E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	3E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	6.5E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-137

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, BETA (BETA-BHC) (319-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	Experimentally measured value (Sahsuvar et al. 2003).	3.5E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.78
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+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.	4.60E+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.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-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).	4.39E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-137

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, BETA (BETA-BHC) (319-85-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	ATSDR Intermediate MRL (ATSDR 2020).	6.0E-04
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.8E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	2.2E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.8E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-138

CHEMICAL-SPECIFIC INPUTS FOR GAMMA-HEXACHLOROCYCLOHEXANE (LINDANE) (58-89-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	Experimentally measured value (Cetin et al. 2006).	2.5E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.72
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+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.	4.60E+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.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-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)	3.96E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-138

CHEMICAL-SPECIFIC INPUTS FOR GAMMA-HEXACHLOROCYCLOHEXANE (LINDANE) (58-89-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.1E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E-03
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.1E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-139

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.53E+00
H (atm·m^3/mol)	Experimentally measured value (Wolfe et al. 1982).	2.7E-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
Log K_{ow} (unitless)	Hansch (1995).	5.04
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.	9.01E+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.	9.01E+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.	6.76E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.80E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.00E+00
t (hr/event)*	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
Health Benchmarks		

TABLE A-1-139

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

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-04
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-140

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.08E+01
H (atm·m^3/mol)	Experimentally measured value (Ashworth et al. 1988).	8.35E-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
Log K_{ow} (unitless)	Hansch (1995).	4.14
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.	2.27E+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.	2.27E+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.	1.71E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.40E+00
t (hr/event)*	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)	*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)	8.68E+02
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	7E-04

TABLE A-1-140

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	4E-02
RfC (mg/m^3)	IRIS (U.S. EPA 20204b).	3E-02
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	3.9E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	9.8

Notes: NA = Not applicable
ND = No data available

TABLE A-1-141

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 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.0E-03
H (atm·m^3/mol)	Calculated value (Zhang et al. 2010).	8.2E-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
Log K_{ow} (unitless)	Hansch (1995).	7.54
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.	1.12E+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.	1.12E+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.	8.40E+04
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.40E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.70E+01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04

TABLE A-1-141

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

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-142

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPROPENE (1888-71-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	248.75
T_m (K)	CRC Handbook (1995)	200.25
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Calculated value (Hilal et al. 2008).	1.0E-02
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	4.38
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for most semivolatile nonionizing organic compounds cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.02E+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.	2.02E+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.	1.52E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.88E+00
t (hr/event)*	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)	--	ND

TABLE A-1-142

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPROPENE (1888-71-7)

Parameter	Reference and Explanation	Value
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* value was calculated by multiplying a food chain multiplier (*FCM*), 1.61, with an estimated *BCF*, 1.26E+03. *BCF*s were estimated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995e).	2.03E+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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-143

CHEMICAL-SPECIFIC INPUTS FOR HEXAHYDRO-1,3,5-TRINITRO-1,3,5-TRIAZINE (121-82-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	6.32E-08
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Sangster (1993).	0.87
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+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.	4.60E+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.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-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)	2.70E+00

TABLE A-1-143

CHEMICAL-SPECIFIC INPUTS FOR HEXAHYDRO-1,3,5-TRINITRO-1,3,5-TRIAZINE (121-82-4)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	8E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	8E-02
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-144

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.07E-02
H (atm·m^3/mol)	Experimentally measured value (ten Hulscher et al. 1992).	3.5E-07
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
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	6.7
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for most semivolatile nonionizing organic compounds cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.86E+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.	3.86E+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.	2.89E+05
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.10E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.20E+00
t (hr/event)*	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
Health Benchmarks		

TABLE A-1-144

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

Parameter	Reference and Explanation	Value
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 1993b).	1E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the Inhalation CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 0.1 (U.S. EPA 1993b).	2E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-145

CHEMICAL-SPECIFIC INPUTS FOR IRON (7439-89-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	55.84
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	1808.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.00E-03
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	7E-01
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

TABLE A-1-145

CHEMICAL-SPECIFIC INPUTS FOR IRON (7439-89-6)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.0E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-146

CHEMICAL-SPECIFIC INPUTS FOR ISOBUTYL ALCOHOL (78-83-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.14
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-02
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+04
H (atm·m^3/mol)	Experimentally measured value (Kim and Kim 2014).	4.49E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Hansch (1995).	0.76
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.	4.79E+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.	4.79E-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.	3.59E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.30E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	5.60E-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)	2.23E+00

TABLE A-1-146

CHEMICAL-SPECIFIC INPUTS FOR ISOBUTYL ALCOHOL (78-83-1)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-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 72 kg.	1E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-147

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+04
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	6.62E-05
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
Log K_{ow} (unitless)	Veith (1980).	1.7
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.	4.69E+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.	4.69E-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.	3.52E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	4.40E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.10E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-01

TABLE A-1-147

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	9.5E-04
RfC (mg/m^3)	CalEPA (2020).	2E+00
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	9.5E-04
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.170E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-148

CHEMICAL-SPECIFIC INPUTS FOR KEPONE (143-50-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	490.68
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.90E-10
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+00
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	5.38E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	5.41
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.	2.08E+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.	2.08E+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.	1.56E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.60E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+02
B	*B* value was obtained from U.S. EPA (1992b).	2.00E+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 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)	5.39E+04
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04

TABLE A-1-148

CHEMICAL-SPECIFIC INPUTS FOR KEPONE (143-50-0)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1E+01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-149

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	207.2
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	600.5
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.43E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.28E-06
Log 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
τ (hr)	--	ND
t (hr/event)*	--	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
Health Benchmarks		
RfD (mg/kg/day)	--	ND

TABLE A-1-149

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

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-150

CHEMICAL-SPECIFIC INPUTS FOR MAGNESIUM (7439-95-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	24.30
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	924.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
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

TABLE A-1-150

CHEMICAL-SPECIFIC INPUTS FOR MAGNESIUM (7439-95-4)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-151

CHEMICAL-SPECIFIC INPUTS FOR MALATHION (121-75-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	Experimentally measured value (Watanabe 1993).	1.5E-08
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	2.36
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+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.	4.60E+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.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-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)	3.66E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-151

CHEMICAL-SPECIFIC INPUTS FOR MALATHION (121-75-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-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 72 kg.	7E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-152

CHEMICAL-SPECIFIC INPUTS FOR MANGANESE (7439-96-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	54.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1517.15
Vp (atm)	--	ND
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)	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.00E-06
Log K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2.4E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5E-05
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND

TABLE A-1-152

CHEMICAL-SPECIFIC INPUTS FOR MANGANESE (7439-96-5)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	U.S. EPA (1996c)	8.00E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-153

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	200.59
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	234.23
Vp (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	2.63E-06 at 25°C
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	5.62E-02
H (atm·m^3/mol)	Experimentally measured value (Andersson et al. 2008).	7.6E-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
Log K_{ow} (unitless)	Daylight (1999).	0.62
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S. EPA (1997g)	1.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	3.00E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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 elemental mercury into the fish tissue.	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	3E-04

TABLE A-1-153

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

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-154

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	2.50E+04
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.810E-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
Log K_{ow} (unitless)	Tanii (1984).	0.68
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.	4.14E+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.	4.14E-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.	3.10E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.80E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.20E-01
t (hr/event)*	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)	1.94E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-154

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	3E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-155

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	2.90E+04
H (atm·m^3/mol)	Experimentally measured value (Vitenberg and Dobryakov 2008).	4.70E-06
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
Log K_{ow} (unitless)	Hansch (1995).	-0.77
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.	2.94E-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.	2.94E-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.	2.21E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.80E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.40E-01
t (hr/event)*	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)	1.53E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E+00
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-155

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E+01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-156

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.84E-02
H (atm·m^3/mol)	Experimentally measured value (Altschuh et al. 1999).	2.0E-07
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
Log K_{ow} (unitless)	Hansch (1995).	5.08
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.10E+01
t (hr/event)*	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)	1.56E+04
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-03
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-156

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	2E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-157

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	8.336E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	0.18
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+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.	4.60E+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.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-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)	8.07E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-157

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	1E+00
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.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-158

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.45E+04
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	7.796E-03
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
Log K_{ow} (unitless)	Hansch (1995).	1.19
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.30E-01
t (hr/event)*	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)	4.72E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-158

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1.4E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-159

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.34E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.246E-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
Log K_{ow} (unitless)	Hansch (1995).	0.91
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.80E-01
t (hr/event)*	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)	2.89E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-159

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	9E-02
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.5E+03

Notes: NA = Not applicable
ND = No data available

TABLE A-1-160

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.40E+05
H (atm·m^3/mol)	Experimentally measured value (Kim and Kim 2014).	9.50E-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
Log K_{ow} (unitless)	Hansch (1995).	0.29
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.	2.03E+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.	2.03E-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.	1.52E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.10E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.40E-01
t (hr/event)*	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)	9.78E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-160

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-161

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 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.00E+04
H (atm·m^3/mol)	Experimentally measured value (Kim and Kim 2014).	2.54E-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
Log K_{ow} (unitless)	Tanii (1986).	1.31
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.	1.31E+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.	1.31E-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.	9.79E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.30E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.60E-01
t (hr/event)*	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)	5.83E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	8E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-161

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	3E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-162

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6) (FISH PATHWAY ONLY)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1997g)	216.0
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	U.S. EPA (1997g)	4.7E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	5.28E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.11E-06
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	0.08
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	U.S. EPA (1997g)	7.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	1.00E+05
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	Defaultτ value cited in U.S. EPA (1997g) for a Trophic Level 4 fish (6.80E+06), multiplied by 15% to adjust for the maximum fraction of total mercury assumed to by methylated in surface water .	1.02E+06
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND

TABLE A-1-162

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6) (FISH PATHWAY ONLY)

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-163

CHEMICAL-SPECIFIC INPUTS FOR METHYL METHACRYLATE (80-62-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	100.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.10E-02
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.60E+04
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.280E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-06
Log K_{ow} (unitless)	Hansch (1995).	1.38
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.	1.48E+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.	1.48E-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.	1.11E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.40E-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_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.59E+00

TABLE A-1-163

CHEMICAL-SPECIFIC INPUTS FOR METHYL METHACRYLATE (80-62-6)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1.4E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	7E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-164

CHEMICAL-SPECIFIC INPUTS FOR METHYL-5-NITROANILINE, 2- (5-NITRO-O-TOLUIDINE) (99-55-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Group Contribution Method described in Hine and Mookerjee (1975).	1.94E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-06
Log K_{ow} (unitless)	Hansch (1995).	1.87
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
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).	1.55E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	2E-02
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	9E-03
RfC (mg/m^3)	--	ND

TABLE A-1-164

CHEMICAL-SPECIFIC INPUTS FOR METHYL-5-NITROANILINE, 2- (5-NITRO-O-TOLUIDINE) (99-55-8)

Parameter	Reference and Explanation	Value
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-165

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)	Experimentally measured value (Rice et al. 1997).	3.8E-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
Log K_{ow} (unitless)	Hansch (1995).	2.86
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.	6.48E+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.	6.48E+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.	4.86E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.40E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	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)	8.78E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2.5E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-165

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	9.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-166

CHEMICAL-SPECIFIC INPUTS FOR 3-METHYLCHOLANTHRENE (56-49-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	5.24E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-06
Log K_{ow} (unitless)	Hansch (1995).	6.42
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.	2.05E+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 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.	2.05E+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.	1.54E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.60E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg $_{FW\ tissue}$)	--	NA

TABLE A-1-166

CHEMICAL-SPECIFIC INPUTS FOR 3-METHYLCHOLANTHRENE (56-49-5)

Parameter	Reference and Explanation	Value
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)	1.10E+06
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020).	2.2E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.2E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-167
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)	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)	Experimentally measured value (Hiatt 2013).	8.076E-04
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
Log K_{ow} (unitless)	Martiska (1990).	1.7
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.	2.66E+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.	2.66E+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).	5.40E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	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)	1.15E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	1E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-167
CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Screening PPRTV (U.S. EPA 2020c).	4E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-168

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)	84.93
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)	Experimentally measured value (Hiatt 2013).	2.462E-03
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
Log K_{ow} (unitless)	Hansch (1995).	1.25
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.	1.17E+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.	1.17E-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.	8.78E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.40E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	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)	5.25E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-03

TABLE A-1-168

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

Parameter	Reference and Explanation	Value
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2E-03
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	6E-01
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	4E-05
MCL	National Primary Drinking Water Regulations.	5.0E-03
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-169

CHEMICAL-SPECIFIC INPUTS FOR 2-METHYLNAPTHALENE (91-57-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	142.20
T_m (K)	CRC Handbook (1995)	307.55
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.786-04
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).	7.84E-06
Log K_{ow} (unitless)	Hansch (1995).	3.86
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.42E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.44E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.87E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.24E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-03
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

TABLE A-1-169

CHEMICAL-SPECIFIC INPUTS FOR 2-METHYLNAPTHALENE (91-57-6)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-170

CHEMICAL-SPECIFIC INPUTS FOR MOLYBDENUM (7439-98-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	95.94
T_m (K)	--	N/A
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	N/A
D_a (cm^2/s)	--	N/A
D_w (cm^2/s)	--	N/A
Log K_{ow} (unitless)	--	N/A
K_{oc} (mL/g)	--	N/A
Kd_s (cm^3/g)	U.S. EPA (1995g)	2.00E+01
Kd_{sw} (L/Kg)	--	2.00E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-03
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

TABLE A-1-170

CHEMICAL-SPECIFIC INPUTS FOR MOLYBDENUM (7439-98-7)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	U.S. EPA (1996c)	2.40E+00

Notes: NA = Not applicable
ND = No data available

TABLE A-1-171

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)	Experimentally measured value (Hiatt 2013).	2.972E-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
Log K_{ow} (unitless)	Hansch (1995)..	3.3
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.30E-01
t (hr/event)*	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)	1.90E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-171

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

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-02
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.2E-01
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	3E-03
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.2E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	6.2E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-172

CHEMICAL-SPECIFIC INPUTS FOR 1,4-NAPHTHAQUINONE (130-15-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	158.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	399.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	1.97E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.98E-06
Log K_{ow} (unitless)	Hansch (1995).	1.71
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.39E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.05E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.93E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.13E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA
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

TABLE A-1-172

CHEMICAL-SPECIFIC INPUTS FOR 1,4-NAPHTHAQUINONE (130-15-4)

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-173

CHEMICAL-SPECIFIC INPUTS FOR 2-NAPHTHYLAMINE (91-59-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	143.18
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	323.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	1.86E-07
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).	8.39E-06
Log K_{ow} (unitless)	Hansch (1995).	2.28
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.	1.74E+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.	1.74E+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.	1.31E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.90E-02
Biotransfer Factors for Animals		

TABLE A-1-173

CHEMICAL-SPECIFIC INPUTS FOR 2-NAPHTHYLAMINE (91-59-8)

Parameter	Reference and Explanation	Value
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)	3.18E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.8E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.8E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-174

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
Log 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. The default value used by DRAS is based on the most neutral pH (6.8).	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). The default value used by DRAS is based on the most neutral pH (6.8).	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
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b)	7.80E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-174

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	CalEPA (2020)	1.4E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	8.6E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.2E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-175

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)	Experimentally measured value (Altschuh et al. 1999).	5.9E-08
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
Log K_{ow} (unitless)	Hansch (1995).	1.85
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.	6.59E+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.	6.59E-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.	4.94E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	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
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	1E-02

TABLE A-1-175

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	--	NA
RfC (mg/m^3)	Screening PPRTV (U.S. EPA 2020c).	5E-05
Inhalation CSF (mg/kg/day)$^{-1}$	--	NA
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-176

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 25°C (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
Log K_{ow} (unitless)	Hansch (1995).	1.37
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.	2.22E+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.	2.22E-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.	1.67E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.57E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.09E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	1E-03

TABLE A-1-176

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

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-177

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)	Experimentally measured value (Altschuh et al. 1999).	1.1E-09
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
Log K_{ow} (unitless)	Hansch (1995).	1.39
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.	2.33E+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.	2.33E-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.	1.74E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.33E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.09E-01
t (hr/event)*	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)	6.71E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	4E-03
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	2E-02

TABLE A-1-177

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

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	6E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	2E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-178

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.92E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.542E-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
Log K_{ow} (unitless)	Hansch (1995).	1.85
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.90E-01
t (hr/event)*	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

TABLE A-1-178

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

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	9E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.70E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-179

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 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+03
H (atm·m^3/mol)	Experimentally measured value (Guo and Bimblecombe 2007).	7.00E-06
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
Log K_{ow} (unitless)	Hansch (1995).	1.79
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.	5.75E+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.	5.75E-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.	4.31E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.12E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.17E-01
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	--	ND

TABLE A-1-179

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

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c). PPRTV value is subchronic.	5E-04
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-180

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)	Experimentally measured value (Tremp et al. 1993).	1.3E-08
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
Log K_{ow} (unitless)	Hansch (1995).	1.91
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.	7.55E+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.	7.55E-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.	5.66E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	6.13E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.17E-01
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-180

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

Parameter	Reference and Explanation	Value
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)	--	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)	U.S. EPA (1995f)	8.28E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-181

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPROPANE (79-46-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	89.09
T_m (K)	U.S. EPA (1995g)	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.40E-02
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.70E+05
H (atm·m^3/mol)	Experimentally measured value (Benes and Dohnal 1999).	1.20E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.23E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.01E-05
Log K_{ow} (unitless)	Chem. Inspect Test Inst. (1992).	0.93
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.	6.53E+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.	6.53E-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.	4.90E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.30E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.40E-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)	3.00E+00

TABLE A-1-181

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPROPANE (79-46-9)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	6E-03
Oral CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	9.4E+00
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-02
Inhalation CSF $(mg/kg/day)^{-1}$	HEAST (U.S. EPA 1997c).	9.4E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-182

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROQUINOLINE-1-OXIDE (56-57-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	190.16
T_m (K)	CRC Handbook (1995)	427.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	2.72E-14
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.00E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	1.09
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.40E-01
t (hr/event)*	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)	--	NA
BAF_{fish} (L/kg FW)	--	NA
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

TABLE A-1-182

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROQUINOLINE-1-OXIDE (56-57-5)

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-183

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIETHYLAMINE (55-18-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	102.14
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	2.60E-03
S (mg/L)	U.S. EPA (1995g)	2.00E+05
H (atm·m^3/mol)	Experimentally measured value (Klein 1982).	1.8E-06
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	0.48
K_{oc} (mL/g)	U.S. EPA (1995g)	3.00E+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 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.	3.00E-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.	2.10E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	9.90E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	6.30E-01
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		

TABLE A-1-183

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIETHYLAMINE (55-18-5)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.5E+02
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.5E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-184

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIMETHYLAMINE (62-75-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.08
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.10E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+06
H (atm·m^3/mol)	Experimentally measured value (Klein 1982).	1.6E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	-0.57
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.	4.24E-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.	4.24E-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.	3.18E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.70E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.70E-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)	2.17E-01

TABLE A-1-184

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIMETHYLAMINE (62-75-9)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	8E-06
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5.1E+01
RfC (mg/m^3)	Screening PPRTV (U.S. EPA 2020c).	4E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5.0E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-185

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 25°C
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
Log K_{ow} (unitless)	Hansch (1995).	2.63
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.	1.45E+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.	1.45E+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.	1.09E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.10E-01
t (hr/event)*	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)	5.87E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND

TABLE A-1-185

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	5.4E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	5.8E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-186

CHEMICAL-SPECIFIC INPUTS FOR NITROSO-DI-N-PROPYLAMINE, N- (621-64-7)

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)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	6.39E-06
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
Log K_{ow} (unitless)	Hansch (1995).	1.36
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.	2.17E+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.	2.17E-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.	1.63E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.40E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	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)	6.36E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-186

CHEMICAL-SPECIFIC INPUTS FOR NITROSO-DI-N-PROPYLAMINE, N- (621-64-7)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	7.0E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	7.0E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-187

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)	Calculated value (Mackay et al. 2006).	1.1E-03
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
Log K_{ow} (unitless)	Hansch (1995).	3.13
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.40E+00
t (hr/event)*	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)	1.41E+02
BAF_{fish} (L/kg, FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	4.9E-03

TABLE A-1-187

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	9.0E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.85E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-188

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMETHYLETHYLAMINE (10595-95-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	88.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.00E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+05
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	2.73E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Vera (1992).	0.04
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.	1.29E+00
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.	1.29E-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.	9.66E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.60E-05
Biotransfer Factors for Animals		

TABLE A-1-188

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMETHYLETHYLAMINE (10595-95-6)

Parameter	Reference and Explanation	Value
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)	6.32E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.20E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.2E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-189

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMORPHOLINE (59-89-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	116.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	302.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	1.41E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.44
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.60E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	6.7E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	6.7E+00

TABLE A-1-189

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMORPHOLINE (59-89-2)

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-190

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPIPERIDINE (100-75-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	114.5
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.90E-04
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.50E+05
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	2.12E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	0.36
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.	2.31E+00
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.	2.31E-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.	1.73E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.30E-04
Biotransfer Factors for Animals		

TABLE A-1-190

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPIPERIDINE (100-75-4)

Parameter	Reference and Explanation	Value
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)	1.12E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	9.4E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	9.4E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-191

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPYRROLIDINE (930-55-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	100.11
T_m (K)	--	
Vp (atm)	*Vp* value cited in Montgomery and Weldom (1991).	2.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.80E+05
H (atm·m^3/mol)	Experimentally measured value (Klein 1982).	6.6E-08
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).	1.04E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.19
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	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 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.	6.50E-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.	4.90E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.40E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.50E-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)	4.22E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-191

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPYRROLIDINE (930-55-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2.1E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2.2E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-192

CHEMICAL-SPECIFIC INPUTS FOR OCTAMETHYLPYROPHOSPHORAMIDE (152-16-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	286.26
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-06
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.00E+06
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	6.31E-17
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).	5.62E-06
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	-1.01
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	3.10E-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.	3.10E-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.	2.30E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-05
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-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).	1.01E-01

TABLE A-1-192

CHEMICAL-SPECIFIC INPUTS FOR OCTAMETHYLPYROPHOSPHORAMIDE (152-16-9)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	2E-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 72 kg.	7E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-193

CHEMICAL-SPECIFIC INPUTS FOR PARATHION (ETHYL) (56-38-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	291.27
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-08
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.50E+00
H (atm·m^3/mol)	Experimentally measured value (Fendinger and Glotfelty 1990).	8.2E-08
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).	5.79E-06
Log K_{ow} (unitless)	Hansch (1995).	3.83
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	5.80E+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.	5.80E+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.	4.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-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)	4.80E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-193

CHEMICAL-SPECIFIC INPUTS FOR PARATHION (ETHYL) (56-38-2)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	6E-03
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 (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.3E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-194

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f)	3.20E-02
H (atm·m^3/mol)	Experimentally measured value (McPhedran et al. 2013).	3.3E-04
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
Log K_{ow} (unitless)	Hansch (1995).	5.17
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.90E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-04

TABLE A-1-194

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Value
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)	US. EPA (1995f)	5.0E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-195

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROETHANE (76-01-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.31
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	244.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	1.607E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.30E-06
Log K_{ow} (unitless)	Hansch (1995).	3.22
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.63E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.05E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.12E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	9E-02
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Route to route extrapolation from Oral CSF.	9E-02
MCL	National Primary Drinking Water Regulations.	ND

TABLE A-1-195

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROETHANE (76-01-7)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-196

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 25°C (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)	Experimentally measured value (Kawamoto and Urano 1989).	3.70E-06
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
Log K_{ow} (unitless)	Sangster (1994).	4.64
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.	5.66E+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.	5.66E+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.	4.24E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.90E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.50E+00
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish}	--	NA

TABLE A-1-196

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Value
(L/kg FW tissue)		
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)	IRIS (U.S. EPA 2020b).	3E-03
Oral CSF $(mg/kg/day)^{-1}$	HEAST (U.S. EPA 1997c).	2.6E-01
RfC (mg/m^3)	--	ND
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.	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-197

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)	Experimentally measured value (Hellmann 1987).	2.4E-08
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
Log K_{ow} (unitless)	Hansch (1995).	5.12
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). The default value used in DRAS is based on a neutral pH.	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. The default value used in DRAS is based on a neutral pH.	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} at a neutral pH that is provided in this table.	4.44E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.90E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.70E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E+01
Biotransfer Factors for Animals		

TABLE A-1-197

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Value
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)	IRIS (U.S. EPA 2020b).	5E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	4E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-198

CHEMICAL-SPECIFIC INPUTS FOR PHENACETIN (62-44-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	179.21
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	407.15 to 408.15
Vp (atm)	--	ND
S (g/1310ml of H_2O)	*S* value cited in U.S. EPA (1995b).	1.0
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	4.80E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.82E-06
Log K_{ow} (unitless)	Nakagawa (1992).	1.58
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.03E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.08E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.80E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.2E-03
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.2E-03

TABLE A-1-198

CHEMICAL-SPECIFIC INPUTS FOR PHENACETIN (62-44-2)

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-199

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)	Experimentally measured value (Lee et al. 2012).	5.52E-05
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
Log K_{ow} (unitless)	Hansch (1995).	4.46
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.	2.42E+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.	2.42E+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.	1.82E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.30E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-199

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-200

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)	Experimentally measured value (Guo and Bimblecombe 2007).	3.55E-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
Log K_{ow} (unitless)	Hansch (1995).	1.46
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). The default value in DRAS corresponds with a neutral pH.	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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.30E-01
t (hr/event)*	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-1-200

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)	7.58E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	CalEPA (2020)	2.0E-01
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-201

CHEMICAL-SPECIFIC INPUTS FOR PHENYL MERCURIC ACETATE (62-38-4)

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 25°C (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
Log K_{ow} (unitless)	Hansch (1995).	0.71
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.	4.99E+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.	4.99E-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.	3.74E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.40E-01
t (hr/event)*	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)	2.04E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-201

CHEMICAL-SPECIFIC INPUTS FOR PHENYL MERCURIC ACETATE (62-38-4)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-05
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-202

CHEMICAL-SPECIFIC INPUTS FOR 1,3-PHENYLENEDIAMINE (108-45-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.6
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.00E-05
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.50E+05
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	1.25E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.88E-06
Log K_{ow} (unitless)	Hansch (1995).	-0.33
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.10E+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.	1.10E-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.	8.25E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	U.S. EPA (1995g)	2.90E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-202

CHEMICAL-SPECIFIC INPUTS FOR 1,3-PHENYLENEDIAMINE (108-45-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-03
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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-203

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
Log K_{ow} (unitless)	Hansch (1995).	3.56
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.	3.16E+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.	3.16E+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.	2.37E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.50E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.40E+00
t (hr/event)*	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
Biotransfer Factors for Animals		

TABLE A-1-203

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Value
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)	2.99E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	2E-04
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-204

CHEMICAL-SPECIFIC INPUTS FOR A-PICOLINE (109-06-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	93.12
T_m (°K)	--	203.15
Vp (mm@°C)	*Vp* value cited in U.S. EPA (1995g).	8.00E+00
S (mg/L)	*S* value cited in U.S. EPA (1995g).	
H (atm·m^3/mol)	Calculated value (Hilal et al. 2008).	2.4E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.50E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.60E-06
Log K_{ow} (unitless)	Hansch (1995).	1.11
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.50E+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.	1.50E+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.	1.12E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.16E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.24E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.76E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.29E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		

TABLE A-1-204

CHEMICAL-SPECIFIC INPUTS FOR A-PICOLINE (109-06-8)

Parameter	Reference and Explanation	Value
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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-205

CHEMICAL-SPECIFIC INPUTS FOR POLYCHLORINATED BIPHENYLS (AROCLORS) (1336-36-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	328
T_m (°K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.00E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	8.00E-02
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Group Contribution Method described in Hine and Mookerjee (1975).	2.23E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
Log K_{ow} (unitless)	Hansch (1995).	6.29
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1998c).	9.83E+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 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.	7.37E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.30E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.30E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-205

CHEMICAL-SPECIFIC INPUTS FOR POLYCHLORINATED BIPHENYLS (AROCLORS) (1336-36-3)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	The BAF_{fish} for PCBs was calculated by multiplying the composite total baseline BAF_{lipids} for trophic level 4 fish from 62 FR 11723, March 12, 1997 (5.27E+07) by the sample-weighted mean lipid content for trophic Level 4 fish (13.19%) cited in Table 2, Appendix 1 in U.S. EPA (1995e).	6.95E+06
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b). Based on *high-risk* Aroclors,(i.e. Aroclor 1254)	2E-05
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	7E-05
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2E+00
MCL	National Primary Drinking Water Regulations.	5E-04
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.4E-02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-206

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
Log K_{ow} (unitless)	Ellington (1988).	3.43
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.	2.35E+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.	2.35E+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.	1.77E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.60E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.20E+00
t (hr/event)*	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)	2.38E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	7.5E-02

TABLE A-1-206

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-207

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)	Experimentally measured value (Lee et al. 2012).	2.40E-05
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
Log K_{ow} (unitless)	Hansch (1995).	4.88
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.50E+00
t (hr/event)*	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)	8.73E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-02
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-207

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-208

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)	Experimentally measured value (Bernauer and Dohnal 2009).	8.97E-06
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
Log K_{ow} (unitless)	Hansch (1995).	0.65
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.	3.92E+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.	3.92E-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.	2.94E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.90E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.70E-01
t (hr/event)*	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)	1.84E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-03
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-208

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-209

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
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	3.45
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for most semivolatile nonionizing organic compounds cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.46E+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.	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+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.50E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.50E-01
t (hr/event)*	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).	2.47E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND

TABLE A-1-209

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2.2E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2.2E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-210

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.96
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.03E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.20E-05
Log 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. The default value in DRAS is based on a neutral pH.	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). The default value in DRAS is based on a neutral pH.	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
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.29E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-03
Oral *CSF* (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-210

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	CalEPA (2020)	2E-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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-211

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.87
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.38E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.71E-06
Log 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. The default value in DRAS is based on a neutral pH.	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). The default value in DRAS is based on a neutral pH.	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
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	8.77E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-03
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-211

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-212

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
Log K_{ow} (unitless)	Hansch (1995).	1.93
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.	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 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.	7.90E-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).	4.10E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.60E+00
t (hr/event)*	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)	1.73E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-212

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-04
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-213

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)	Experimentally measured value (Kim and Kim 2014).	3.69E-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
Log K_{ow} (unitless)	Hansch (1995).	2.95
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.80E-01
t(hr/event)*	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)	1.03E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-213

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1E-01
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-214

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 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.30E+00
H (atm·m^3/mol)	Experimentally measured value (McPhedran et al. 2013).	5.6E-04
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
Log K_{ow} (unitless)	Hansch (1995).	4.64
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.	5.66E+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 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.	5.66E+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.	4.24E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.80E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.80E+00
*t** (hr/event)	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-214

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Value
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)	IRIS (U.S. EPA 2020b).	3E-04
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)	5.0E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-215

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 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	1.93E-05
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	5.00E-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
Log K_{ow} (unitless)	Shiu (1998).	6.8
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.	2.91E+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 organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.91E+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. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.18E+04
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.40E+00
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.10E+00
*t** (hr/event)	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 $_{\text{FW tissue}}$)	--	NA

TABLE A-1-215

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8 -TETRACHLORODIBENZO (P) DIOXIN (1746-01-6)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	The BAF_{fish} for dioxin was calculated by multiplying the composite total baseline BAF_{lipids} for trophic level 4 fish from Table 10 in U.S. EPA (1995e) (9.0E+06) by the sample-weighted mean lipid content for trophic Level 4 fish (13.19%) cited in Table 2, Appendix 1 in U.S. EPA (1995e).	1.19E+06
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	7E-10
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.3E+05
RfC (mg/m^3)	CalEPA (2020)	4E-08
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.3E+05
MCL	National Primary Drinking Water Regulations.	3.0E-08
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.0 E-08

Notes: NA = Not applicable
ND = No data available

TABLE A-1-216

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)	Experimentally measured value (Hiatt 2013).	2.065E-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
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e).	2.93
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for VOCs, chlorinated benzenes, and certain chlorinated pesticides as cited in U.S. EPA (1996a). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.50E+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.	2.50E+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.	1.88E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.30E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.20E-01
*t** (hr/event)	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).	9.93E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-02

TABLE A-1-216

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2.6E-02
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2.7E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-217

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.07E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.959E-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
Log K_{ow} (unitless)	Hansch (1995).	2.39
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.20E-01
t (hr/event)*	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)	*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)	3.86E+01
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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-02

TABLE A-1-217

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	2E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	2E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	4.2E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-218

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.32E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	9.919E-03
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
Log K_{ow} (unitless)	Hansch (1995).	3.4
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	9.00E-01
t (hr/event)*	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)	2.26E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-218

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	6E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	2.1E-03
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	4E-02
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	9.4E-04
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.2E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-219

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)	Calculated value (Zhang et al. 2010).	2.4E-04
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
Log K_{ow} (unitless)	Hansch (1995).	4.45
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). The default value in DRAS is based on a neutral pH.	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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.30E+00
t (hr/event)*	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
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA

TABLE A-1-219

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Value
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)	2.51E+03
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-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 72 kg.	1E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-220

CHEMICAL-SPECIFIC INPUTS FOR TETRAETHYL DITHIOPYROPHOSPHATE (SULFOTEP) (3689-24-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	322.31
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.30E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.50E+01
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	4.45E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Tomlin (1994).	3.99
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	5.80E+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 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.	5.80E+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.	4.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	2.80E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-220

CHEMICAL-SPECIFIC INPUTS FOR TETRAETHYL DITHIOPYROPHOSPHATE (SULFOTEP) (3689-24-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-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 72 kg.	2E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-221

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	204.38
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.34E-06
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S. EPA (1996a). The default value in DRAS is based on a neutral pH.	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). The default value in DRAS is based on a neutral pH.	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.00E+04
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	1E-05
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND

TABLE A-1-221

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-222

CHEMICAL-SPECIFIC INPUTS FOR THIONAZIN (297-97-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	248.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	271.45
Vp (mmHg)	U.S. EPA (1995g)	3.00E-03
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	8.60E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	1.86
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.86E+00
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
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

TABLE A-1-222

CHEMICAL-SPECIFIC INPUTS FOR THIONAZIN (297-97-2)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-223

CHEMICAL-SPECIFIC INPUTS FOR TIN (7440-31-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	118.69
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	505.05
Vp (atm)	--	ND
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).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	6E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-223

CHEMICAL-SPECIFIC INPUTS FOR TIN (7440-31-5)

Parameter	Reference and Explanation	Value
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-224

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)	Experimentally measured value (Kim and Kim 2014).	6.65E-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
Log K_{ow} (unitless)	Hansch (1995).	2.73
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.20E-01
t (hr/event)*	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)	7.00E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-224

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5E+00
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-1-225

CHEMICAL-SPECIFIC INPUTS FOR 2,4-TOLUENEDIAMINE (95-80-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	122.17
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.50E+03
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Group Contribution Method described in Hine and Mookerjee (1975).	9.52E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.05E-06
Log K_{ow} (unitless)	Debnath (1992).	0.14
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.50E+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.	2.50E-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.	1.88E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.60E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	4.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-04
Biotransfer Factors for Animals		
BCF_{fish} (unitless FW tissue)	U.S. EPA (1995g)	4.60E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-225

CHEMICAL-SPECIFIC INPUTS FOR 2,4-TOLUENEDIAMINE (95-80-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	4.0E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	CalEPA (2020)	4.0E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-226

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)	Experimentally measured value (Altschuh et al. 1999).	2.06E-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
Log K_{ow} (unitless)	Hansch (1995).	1.32
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.	1.99E+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 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.	1.99E-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.	1.49E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	3.80E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	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)	5.93E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	NA
Oral CSF (mg/kg/day)$^{-1}$	PPRTV (U.S. EPA 2020c).	1.6E-02

TABLE A-1-226

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	NA
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	1.8E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-227

CHEMICAL-SPECIFIC INPUTS FOR P-TOLUIDINE (106-49-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.15
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	317.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.60E+03
H (atm·m^3/mol)	Experimentally measured value (Altschuh et al. 1999).	7.6E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.97E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.43E-06
Log K_{ow} (unitless)	Hansch (1995).	1.39
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.40E+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.	2.40E-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.	1.80E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	3.50E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		

TABLE A-1-227

CHEMICAL-SPECIFIC INPUTS FOR P-TOLUIDINE (106-49-0)

Parameter	Reference and Explanation	Value
RfD (mg/kg/day)	Screening PPRTV (U.S. EPA 2020c).	4E-03
Oral CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	3E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	1E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	3E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-228

CHEMICAL-SPECIFIC INPUTS FOR TOXAPHENE (CHLORINATED CAMPHENES) (8001-35-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	414
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	350.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.79E-01
H (atm·m^3/mol)	Experimentally measured value (Murphy et al. 1987).	6.00E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.34E-06
Log K_{ow} (unitless)	EPI Suite Estimation (U.S. EPA 2020e). Median value selected.	5.9
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.60E+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.	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.	1.95E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.60E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.90E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+02
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	(U.S. EPA 1995g)	2.10E+06

TABLE A-1-228

CHEMICAL-SPECIFIC INPUTS FOR TOXAPHENE (CHLORINATED CAMPHENES) (8001-35-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	9E-05
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.1E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.2E+00
MCL	National Primary Drinking Water Regulations.	3E-03
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	2E-04

Notes: NA = Not applicable
ND = No data available

TABLE A-1-229

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	3.07E+01
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	9.232E-04
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
Log K_{ow} (unitless)	Hansch (1995).	4.02
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	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 $_{FW\ tissue}$)	--	NA

TABLE A-1-229

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Value
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)	8.79E+02
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-02
Oral CSF $(mg/kg/day)^{-1}$	PPRTV (U.S. EPA 2020c).	2.9E-02
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	2E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	2.9E-02
MCL	National Primary Drinking Water Regulations.	7E-02
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.11E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-230

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)	Experimentally measured value (Hiatt 2013).	1.43E-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
Log K_{ow} (unitless)	Hansch (1995).	2.49
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.70E-02
t (hr/event)*	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)	4.60E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-230

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E+00
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	5E+00
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-231

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.40E+03
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	7.080E-04
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
Log K_{ow} (unitless)	Hansch (1995).	1.89
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
τ (hr)	τ value was obtained from U.S. EPA (1992b).	5.70E-01
t (hr/event)*	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)	1.61E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-231

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5.7E-02
RfC (mg/m^3)	Screening PPRTV (U.S. EPA 2020c).	2E-04
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	5.8E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	9.40E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-232

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)	Experimentally measured value (Hiatt 2013).	8.314E-03
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
Log K_{ow} (unitless)	Hansch (1995).	2.42
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.	9.88E+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.	9.88E-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.	7.41E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.60E-01
τ (hr)	τ value was obtained from U.S. EPA (1992b).	8.70E-02
t (hr/event)*	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)	4.07E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04

TABLE A-1-232

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Value
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	4.6E-02
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.5E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	3.5E+02

Notes: NA = Not applicable
ND = No data available

TABLE A-1-233

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (76-13-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.38
T_m (°K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.80E-01
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.70E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	4.814E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.20E-06
Log K_{ow} (unitless)	Hansch (1995).	3.16
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.30E+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 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.	1.30E+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.	9.81E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.40E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+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)	1.48E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-233

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (76-13-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E+01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	PPRTV (U.S. EPA 2020c).	5E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-234

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)	Experimentally measured value (Hiatt 2013).	3.512E-02
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
Log K_{ow} (unitless)	Hansch (1995).	2.53
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.	1.21E+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.	1.21E+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.	9.06E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	1.70E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.00E-01
t (hr/event)*	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)	4.93E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-234

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	HEAST (U.S. EPA 1997c).	7E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-235

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)	Calculated value (Fogg and Sangster 2003).	2.1E-05
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
Log K_{ow} (unitless)	Hansch (1995).	3.72
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). The default value used in DRAS is based on a neutral pH.	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. The default value used in DRAS is based on a neutral pH.	1.60E+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.	1.20E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	7.00E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.40E+00
t (hr/event)*	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
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)	3.96E+02

TABLE A-1-235

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-01
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-236

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)	Calculated value (Zhang et al. 2010).	3.5E-04
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
Log K_{ow} (unitless)	Hansch (1995).	3.69
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). The default value used in DRAS is based on a neutral pH.	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. The default value used in DRAS is based on a neutral pH.	3.81E+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.	2.86E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	5.00E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.40E+00
t (hr/event)*	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
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)	3.75E+02

TABLE A-1-236

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	PPRTV (U.S. EPA 2020c).	1E-03
Oral CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	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 72 kg.	4E-03
Inhalation CSF $(mg/kg/day)^{-1}$	IRIS (U.S. EPA 2020b).	1.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.2E+00

Notes: NA = Not applicable
ND = No data available

TABLE A-1-237

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROPHENOXY PROPIONIC ACID (SILVEX) (93-72-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	269.51
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	6.80E-09
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.40E+02
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	9.06E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	3.8
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.30E+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.	2.30E+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.	1.71E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.90E+01
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)	4.55E+02

TABLE A-1-237

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROPHENOXY PROPIONIC ACID (SILVEX) (93-72-1)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	8E-03
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.	5E-02
Aquatic TRV (µg/l)	--.	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-238

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOXYACETIC ACID (93-76-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	255.49
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	9.10E-10
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.80E+02
H (atm·m^3/mol)	Calculated value (Mackay et al. 2006).	5.8E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	3.31
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	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		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.20E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.00E-01
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)	1.93E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-238

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOXYACETIC ACID (93-76-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	1E-02
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 (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-239

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)	Experimentally measured value (Hiatt 2013).	2.331E-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
Log K_{ow} (unitless)	Chem Inspect Test Inst. (1992).	2.27
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.	7.52E+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.	7.52E-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.	5.64E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	9.50E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	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)	3.13E+01
BAF_{fish} (L/kg FW	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	4E-03
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	3E+01

TABLE A-1-239

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	3E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-240

CHEMICAL-SPECIFIC INPUTS FOR O,O,O-TRIETHYLPHOSPHOROTHIATE (126-68-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	198.22
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	2.70E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.17E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.23E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	2.64
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.42E+00
t (hr/event)*	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)	--	ND
BAF_{fish} (L/kg FW)	--	ND
Health Benchmarks		
RfD (water) (mg/kg/day)	--	ND
RfD (food) (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND

TABLE A-1-240

CHEMICAL-SPECIFIC INPUTS FOR O,O,O-TRIETHYLPHOSPHOROTHIATE (126-68-1)

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

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

TABLE A-1-241

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
Log K_{ow} (unitless)	Hansch (1995).	1.18
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.	1.03E+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.	1.03E-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.	7.73E-01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	6.57E-04
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.75E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-02

TABLE A-1-241

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Value
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

Notes: NA = Not applicable
ND = No data available

TABLE A-1-242

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)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	2.08E-8
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
Log K_{ow} (unitless)	Hansch (1995).	1.6
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.	2.22E+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.	2.22E-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.	1.66E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.31E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.75E+00
t (hr/event)*	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
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	5E-04

TABLE A-1-242

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	3E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 72 kg.	2E-03
Inhalation CSF (mg/kg/day)$^{-1}$	Route to route extrapolation from Oral CSF.	3E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-243

CHEMICAL-SPECIFIC INPUTS FOR TRIS(2,3-DIBROMOPROPYL) PHOSPHATE B19 (126-72-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	697.93
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.00E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.70E+00
H (atm·m^3/mol)	EPI Suite calculated value using vapor pressure and water solubility values per Meylan and Howard (1991).	2.18E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.50E-03
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.66E-06
Log K_{ow} (unitless)	Sangster (1994).	4.29
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.80E+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.	2.80E+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.	2.10E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.30E-05
τ (hr)	τ value was obtained from U.S. EPA (1992b).	1.60E+03
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E+03
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA

TABLE A-1-243

CHEMICAL-SPECIFIC INPUTS FOR TRIS(2,3-DIBROMOPROPYL) PHOSPHATE B19 (126-72-7)

Parameter	Reference and Explanation	Value
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)	1.60E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.3E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2020)	2.3E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-244

CHEMICAL-SPECIFIC INPUTS FOR VANADIUM (7440-62-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	50.94
T_m (K)	--	
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	N/A
K_{oc} (mL/g)	--	N/A
Kd_s (cm^3/g)	U.S. EPA (1995g)	5.00E+01
Kd_{sw} (L/Kg)	--	5.00E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b). Value derived from the RfD for vanadium pentoxide.	5E-03
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	ATSDR MRL (ATSDR 2020).	1E-04
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND

TABLE A-1-244

CHEMICAL-SPECIFIC INPUTS FOR VANADIUM (7440-62-2)

Parameter	Reference and Explanation	Value
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.9E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-245

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	50.94
T_m (K)	--	
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	EPI Suite estimated value calculated using the Bond Contribution Methodology described in Hine and Mookerjee (1975) and updated/expanded in Meylan and Howard (1991).	1.17E-03
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	Hansch (1995).	0.73
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.	4.53E+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.	4.53E-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.	3.40E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
τ (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		

TABLE A-1-245

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Value
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)	2.11E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	HEAST (U.S. EPA 1997c).	1E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	2E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.9E+01

Notes: NA = Not applicable
ND = No data available

TABLE A-1-246

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+02
H (atm·m^3/mol)	Experimentally measured value (Hiatt 2013).	2.511E-02
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
Log K_{ow} (unitless)	Sakuratani (2007).	1.46
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for VOCs, chlorinated benzenes, and certain chlorinated pesticides as cited in U.S. EPA (1996a). 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 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.	1.72E+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).	9.20E-03
τ (hr)	τ value was obtained from U.S. EPA (1992b).	2.10E-01
t (hr/event)*	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)	*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).	7.58E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-03

TABLE A-1-246

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Value
Oral CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	7.2E-01
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-01
Inhalation CSF (mg/kg/day)$^{-1}$	IRIS (U.S. EPA 2020b).	1.6E-02
MCL	National Primary Drinking Water Regulations.	2E-03
Aquatic TRV (ug/l)	--	ND

Notes: NA = Not applicable
ND = No data available

TABLE A-1-247

CHEMICAL-SPECIFIC INPUTS FOR XYLENES (TOTAL) (1330-20-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.17
T_m (°K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-02
S (mg/L)	Yalkowsky and Dannenfelser (1992).	1.06E+02
H (atm·m^3/mol)	Experimentally measured value (Kim and Kim 2014).	7.7E-03
D_a (cm^2/s)	D_a value was obtained from WATER9 database (U.S. EPA 2006b).	7.37E-02
D_w (cm^2/s)	D_w value was obtained from WATER9 database (U.S. EPA 2006b).	9.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.16
K_{oc} (mL/g)	K_{oc} value cited in EPI Suite (U.S. EPA 2020e).	3.8E+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 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.	3.8E+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+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.60E-02
τ (hr)	τ value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	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)	Mean value of measured *BCF* values for the three xylene isomers from Ogata et al. (1984).	1.46E+01
BAF_{fish} (L/kg FW)	--	NA

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CHEMICAL-SPECIFIC INPUTS FOR XYLENES (TOTAL) (1330-20-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	2E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	IRIS (U.S. EPA 2020b).	1E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E+01
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.80E+00

Notes: NA = Not applicable
ND = No data available

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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
Log 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
τ (hr)	--	ND
t^* (hr/event)	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	2.06E+03
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	IRIS (U.S. EPA 2020b).	3E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND

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CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Value
RfC (mg/m^3)	--	ND
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

Notes: NA = Not applicable
ND = No data available