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United States
Environmental Protection
Agency

Solid Waste and
Emergency Response
(5305W)

EPA530-D-99-001B
August 1999
www.epa.gov/osw

Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities

Volume Two
Appendix A

Peer Review Draft

US EPA ARCHIVE DOCUMENT

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APPENDIX A

CHEMICAL-SPECIFIC DATA

Screening Level Ecological Risk Assessment Protocol

August 1999

A-1 CHEMICALS FOR CONSIDERATION AS COMPOUNDS OF POTENTIAL CONCERN

A-2 COMPOUND SPECIFIC PARAMETER VALUES

US EPA ARCHIVE DOCUMENT

APPENDIX A-1

INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

US EPA ARCHIVE DOCUMENT

TABLE A-1
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50-00-0	Formaldehyde (methylene oxide)	K009, K010, K038, K040, K156, K157	X		X	X	
50-06-6	Phenobarbital						
50-07-7	Mitomycin						
50-18-0	Cyclophosphamide						
50-29-3	4,4'-DDT		X				
50-32-8	Benzo(a)pyrene	F032, F034, F037, F038, K001, K022, K035, K141, K142, K144, K145, K147, K148	X		X	X	X
50-55-5	Reserpine						
51-28-5	2,4-Dinitrophenol	K001	X			X	
51-43-4	Epinephrine						
51-52-5	Propylthiouracil						
51-79-6	Ethyl carbamate (urethane)					X	
52-85-7	Famphur						
53-70-3	Dibenzo(a,h)anthracene	F032, F034, K022, K141, K142, K144, K145, K147, K148	X			X	
53-96-3	2-Acetylaminofluorene						
54-11-5	Nicotine						
55-18-5	Nitrosodiethylamine						
55-38-9	Fenthion						
55-63-0	Nitroglycerine						
55-91-4	Diisopropylfluorophosphate (DFP)						
56-04-2	Methylthiouracil						

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US EPA ARCHIVE DOCUMENT

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56-23-5	Carbon tetrachloride	F001, F024, F025, K016, K019, K020, K021, K073, K116, K150, K151, K157	X		X	X	X
56-38-2	Parathion						
56-49-5	3-Methylcholanthrene						
56-53-1	Diethylstilbestrol						
56-55-3	Benzo(a)anthracene	F032, F034, K001, K022, K035, K141, K142, K143, K144, K145, K147, K148	X		X	X	
56-57-5	Nitroquinoline-1-oxide						
56-72-4	Coumaphos						
57-12-5	Cyanide		X				X
57-14-7	1,1-Dimethyl hydrazine	K107, K108, K109, K110					
57-24-9	Strychnine		X			X	
57-41-0	5,5-Diphenylhydantoin						
57-57-8	beta-Propiolactone						
57-74-9	Chlordane	K097	X			X	
57-97-6	7,12-Dimethylbenz(a)anthracene						
58-89-9	gamma-BHC (Lindane)						
58-89-9	Lindane (all isomers)					X	
58-90-2	2,3,4,6-Tetrachlorophenol	F020, F023, F027, F028, K001	X				
59-50-7	4-Chloro-3-methylphenol (p-chloro-m-cresol)	F004, K001					
59-89-2	N-Nitrosomorpholine						
60-09-3	Aminoazobenzene						
60-11-7	Dimethyl aminoazobenzene					X	

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60-34-4	Methyl hydrazine						
60-35-5	Acetamide						
60-51-5	Dimethoate						
60-57-1	Dieldrin		X				
61-82-5	Amitrole						
62-38-4	Phenylmercury acetate						
62-44-2	Phenacetin						
62-50-0	Ethyl methanesulfonate		X			X	
62-53-3	Aniline	K083, K103, K104, K112, K113	X			X	
62-55-5	Thioacetamide						
62-56-6	Thiourea						
62-73-7	Dichlorovos		X				
62-74-8	Fluoroacetic acid, sodium salt						
62-75-9	N-Nitrosodimethylamine						
63-25-2	Carbaryl	K156					
64-17-5	Ethanol						
64-18-6	Formic acid (methanoic acid)	K009, K010	X			X	
64-64-7	Di-n-propylnitrosamine					X	
64-67-5	Diethyl sulfate						
65-85-0	Benzoic acid		X				X
66-27-3	Methyl methanesulfonate						
66-75-1	Uracil mustard						

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67-56-1	Methanol		X				
67-64-1	Acetone		X				X
67-66-3	Chloroform (trichloromethane)	F024, F025, K009, K010, K019, K020, K021, K029, K073, K116, K149, K150, K151, K158	X		X	X	X
67-72-1	Hexachloroethane (perchloroethane)	F024, F025, K016, K030, K073	X		X	X	
68-12-2	Dimethyl formamide						
70-25-7	N-Methyl-N'-nitro-N-nitrosoguanidine (MNNG)						
70-30-4	Hexachlorophene		X			X	
71-43-2	Benzene	F005, F024, F025, F037, F038, K085, K104, K105, K141, K142, K143, K144, K145, K147, K151, K159	X		X	X	X
71-55-6	Methyl chloroform (1,1,1-trichloroethane)	F001, F002, F024, F025, K019, K020, K028, K029, K096			X	X	X
72-20-8	Endrin		X				
72-33-3	Mestranol						
72-43-5	Methoxychlor		X			X	
72-54-8	4,4'-DDD		X				
72-55-9	DDE		X			X	
72-57-1	Trypan blue						
74-83-9	Bromomethane (methylbromide)	K131, K132	X		X	X	X
74-87-3	Chloromethane (methyl chloride)	F024, F025, K009, K010, K149, K150, K157	X		X	X	X
74-88-4	Methyl iodide (Iodomethane)						
74-90-8	Hydrogen cyanide	K011, K013					

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74-93-1	Thiomethanol						
74-95-3	Methylene bromide		X		X	X	
74-97-5	Bromochloromethane				X	X	X
75-00-3	Chloroethane		X			X	
75-01-4	Vinyl chloride	F024, F025, K019, K020, K028, K029	X		X	X	X
75-05-8	Acetonitrile	K011, K013, K014	X		X		
75-07-0	Acetaldehyde		X			X	
75-09-2	Methylene chloride	F001, F002, F024, F025, K009, K010, K156, K157, K158	X			X	X
75-15-0	Carbon disulfide	F005	X		X	X	X
75-21-8	Ethylene oxide		X			X	
75-25-2	Bromoform		X			X	X
75-27-4	Bromodichloromethane		X		X	X	X
75-29-6	2-Chloropropane		X			X	
75-34-3	1,1-Dichloroethane	F024, F025	X		X	X	X
75-35-4	1,1-Dichloroethene	F024, F025, K019, K020, K029	X		X	X	
75-36-5	Acetyl chloride						
75-44-5	Phosgene (hydrogen phosphide)	K116				X	
75-45-6	Chlorodifluoromethane		X				X
75-55-8	1,2-Propylenimine (2-methyl aziridine)						
75-56-9	Propylene oxide						
75-60-5	Cacodylic acid						

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75-69-4	Trichlorofluoromethane (Freon 11)	F001, F002	X			X	X
75-70-7	Trichloromethanethiol						
75-71-8	Dichlorodifluoromethane		X			X	
75-86-5	2-Methylactonitrile						
75-87-6	Chloral						
76-01-7	Pentachloroethane	F024, F025					X
76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane(Freon 113)	F001, F002	X			X	X
76-44-8	Heptachlor	K097	X			X	
77-47-4	Hexachlorocyclopentadiene	F024, F025, K032, K033, K034	X			X	X
77-78-1	Dimethyl sulfate	K131				X	
78-00-2	Tetraethyl lead						
78-32-0	Tri-p-tolyl phosphate						
78-34-2	Dioxathion						
78-59-1	Isophorone		X				
78-83-1	Isobutyl alcohol	F005					
78-87-5	1,2-Dichloropropane		X			X	X
78-93-3	2-Butanone (methyl ethyl ketone)	F005	X		X	X	X
78-97-7	2-Hydroxypropionitrile						
79-00-5	1,1,2-Trichloroethane	F002, F024, F025, K019, K020, K095, K096	X		X	X	X
79-01-6	Trichloroethene	F001, F002, F024, F025, K018, K019, K020	X		X	X	X
79-06-1	Acrylamide	K014					

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79-10-7	Acrylic acid						
79-11-8	Chloroacetic acid						
79-19-6	Thiosemicarbazide						
79-20-9	Methyl acetate		X				
79-22-1	Methyl chlorocarbonate						
79-34-5	1,1,2,2-Tetrachloroethane	F024, F025, K019, K020, K030, K073, K095, K150	X		X	X	
79-44-7	Dimethyl carbamoyl chloride						
79-46-9	2-Nitropropane	F005					
80-62-6	Methyl methacrylate						
81-07-2	Saccharin						
81-81-2	Warfarin						
82-68-8	Pentachloronitrobenzene (PCNB)		X			X	
83-32-9	Acenaphthene	K022	X				
84-66-2	Diethyl phthalate		X			X	X
84-74-2	Dibutyl phthalate		X		X	X	X
85-01-8	Phenanthrene	K022					
85-44-9	Phthalic anhydride (1,2-benzenedicarboxylic anhydride)	K023, K024, K093, K094	X			X	
85-68-7	Butylbenzyl phthalate		X		X	X	X
86-30-6	N-Nitrosodiphenylamine		X				
86-50-0	Azinphos-methyl						
86-73-7	Fluorene	K022	X		X		

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86-88-4	alpha-Naphthylthiourea						
87-65-0	2,6-Dichlorophenol	K043					
87-68-3	Hexachlorobutadiene (perchlorobutadiene)	F024, F025, K016, K018, K030	X		X	X	X
87-86-5	Pentachlorophenol	F021, F027, F028, F032, K001	X		X	X	X
88-06-2	2,4,6-Trichlorophenol	F020, F023, F027, F028, K001, K043, K099, K105	X		X	X	X
88-74-4	o-Nitroaniline (2-nitroaniline)					X	
88-75-5	2-Nitrophenol						X
88-85-7	Dinoseb						
90-04-0	o-Anisidine					X	
90-13-1	1-Chloronaphthalene						
91-20-3	Naphthalene	F024, F025, F034, K001, K022, K035, K060, K087, K145	X		X	X	X
91-22-5	Quinoline		X			X	
91-57-6	2-Methylnaphthalene						
91-58-7	2-Chloronaphthalene		X			X	
91-59-8	2-Naphthylamine (beta-naphthylamine)						
91-80-5	Methapyrilene						
91-94-1	3,3'-Dichlorobenzidine		X			X	
92-52-4	Biphenyl		X		X	X	
92-67-1	4-Aminobiphenyl						
92-87-5	Benzidine		X				
92-93-3	4-Nitrobiphenyl						

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93-72-1	Silvex	F027					
94-58-6	Dihydrosaffrole						
94-59-7	Safrole (5-(2-Propenyl)-1,3-benzodioxole)		X			X	
94-75-7	2,4-D		X			X	
95-06-7	Sulfallate						
95-47-6	o-Xylene (dimethyl benzene)		X		X	X	X
95-48-7	o-Cresol	F004	X			X	
95-50-1	1,2-Dichlorobenzene	F002, F024, F025, K042, K085, K105	X		X	X	X
95-53-4	o-Toluidine	K112, K113, K114	X			X	
95-57-8	2-Chlorophenol	K001	X			X	X
95-79-4	5-Chloro-2-methylaniline						
95-80-7	2,4-Toluene diamine	K112, K113, K114, K115, K027					
95-83-0	4-Chloro-1,2-phenylenediamine						
95-94-3	1,2,4,5-Tetrachlorobenzene	K085, K149, K150, K151	X		X	X	X
95-95-4	2,4,5-Trichlorophenol	F020, F023, F027, F028, K001	X		X	X	
96-09-3	Styrene oxide						
96-12-8	1,2-Dibromo-3-chloropropane		X		X	X	
96-18-4	1,2,3-Trichloropropane		X			X	
96-23-1	1,3-Dichloro-2-propanol						
96-45-7	Ethylene thiourea	K123, K124, K125, K126	X			X	
97-63-2	Ethyl methacrylate		X			X	
98-01-1	Furfural		X			X	

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98-07-7	Benzotrichloride	K015, K149	X			X	
98-82-8	Cumene		X		X	X	X
98-83-9	Methyl styrene (mixed isomers)		X			X	
98-86-2	Acetophenone		X			X	X
98-87-3	Benzal chloride						
98-95-3	Nitrobenzene	F004, K083, K103, K104	X			X	
99-09-2	3-Nitroaniline						
99-35-4	1,3,5-Trinitrobenzene		X			X	
99-55-8	5-Nitro-o-toluidine						
99-59-2	5-Nitro-o-anisidine						
99-65-0	1,3-Dinitrobenzene	K025	X			X	
100-01-6	4-Nitroaniline (p-nitroaniline)						
100-02-7	4-Nitrophenol (p-nitrophenol)					X	
100-25-4	1,4-Dinitrobenzene (p-dinitrobenzene)		X			X	
100-41-4	Ethylbenzene		X		X	X	X
100-42-5	Styrene		X		X	X	
100-44-7	Benzyl chloride	K015, K085, K149	X		X	X	
100-51-6	Benzyl alcohol						
100-52-7	Benzaldehyde		X		X	X	X
100-75-4	N-Nitrosopiperidine						
101-05-3	Anilazine						
101-14-4	4,4'-Methylenebis (2-chloroaniline)						

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101-27-9	Barban						
101-55-3	4-Bromophenyl phenyl ether						
101-61-1	4,4'-Methylenebis (N,N-dimethylaniline)						
101-68-8	Methylene diphenyl diisocyanate (MDI)						
101-79-9	4,4-Methylenedianiline					X	
101-80-4	4,4'-Oxydianiline						
102-82-9	Tributylamine						
103-33-3	Azobenzene		X		X	X	
103-85-5	Phenylthiourea						
105-60-2	Caprolactam						
105-67-9	2,4-Dimethylphenol	K001	X			X	X
106-42-3	p-Xylene (dimethyl benzene)				X	X	X
106-44-5	p-Cresol (4-methyl phenol)	F004	X			X	
106-46-7	1,4-Dichlorobenzene	F024, F025, K085, K105, K149, K150	X		X	X	X
106-47-8	p-Chloroaniline		X			X	
106-49-0	p-Toluidine	K112, K113, K114	X			X	
106-50-3	p-Phenylenediamine						
106-51-4	Quinone					X	
106-88-7	1,2-Epoxybutane						
106-89-8	Epichlorohydrin (1-chloro-2,3 epoxypropane)	K017	X			X	
106-93-4	Ethylene dibromide	K117, K118, K136	X			X	
106-99-0	1,3-Butadiene				X	X	

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107-02-8	Acrolein		X			X	
107-05-1	Allyl chloride	F024, F025					
107-06-2	1,2-Dichloroethane (ethylene dichloride)	F024, F025, K018, K019, K020, K029, K030, K096	X		X	X	X
107-07-3	2-Chloroethanol						
107-10-8	n-Propylamine						
107-12-0	Propionitrile						
107-13-1	Acrylonitrile	K011, K013	X		X	X	
107-18-6	Allyl alcohol						
107-19-7	Propargyl alcohol		X			X	
107-20-0	Chloroacetaldehyde	K010					
107-21-1	Ethylene glycol (1,2-ethanediol)		X			X	
107-30-2	Chloromethyl methyl ether						
107-49-3	Tetraethyl pyrophosphate						
107-98-2	Propylene glycol monomethyl ether		X			X	
108-05-4	Vinyl acetate		X			X	
108-10-1	Methyl isobutyl ketone		X			X	X
108-18-9	Diisopropylamine						
108-31-6	Maleic anhydride	K023, K093					
108-38-3	m-Xylene (dimethyl benzene)		X		X	X	X
108-39-4	m-Cresol	F004	X			X	
108-46-3	Resorcinol						

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108-60-1	bis (2-Chloroisopropyl)ether					X	
108-67-8	1,3,5-Trimethylbenzene		X				X
108-87-2	Methylcyclohexane					X	
108-88-3	Toluene	F005, F024, F025, K015, K036, K037, K149, K151	X		X	X	X
108-90-7	Chlorobenzene	F002, F024, F025, K015, K105, K149	X		X	X	X
108-95-2	Phenol	K001, K022, K087	X		X	X	X
108-98-5	Thiophenol (benzenethiol)						
109-06-8	2-Picoline	K026					
109-77-3	Malononitrile		X			X	
109-88-4	2-Methoxyethanol		X			X	
109-89-7	Diethylamine						
109-99-9	Tetrahydrofuran		X				X
110-54-3	n-Hexane		X			X	
110-75-8	2-Chloroethylvinyl ether						
110-80-5	Ethylene glycol monoethyl ether	F005	X			X	
110-86-1	Pyridine	F005, K026, K157	X			X	
111-15-9	Ethylene glycol monoethyl ether acetate					X	
111-42-2	Diethanolamine						
111-44-4	bis(2-chloroethyl)ether	K017	X		X	X	
111-54-6	Ethylene(bis)dithiocarbamic acid						
111-76-2	Ethylene glycol monobutyl ether					X	
111-91-1	bis(2-chloroethoxy)methane				X	X	

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US EPA ARCHIVE DOCUMENT

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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114-26-1	Propoxur (Bayton)						
115-02-6	Azaserine						
115-29-7	Endosulfan		X				
115-90-2	Fensulfothion						
116-06-3	Aldicarb						
117-79-3	2-Aminoanthraquinone						
117-80-6	Dichlone						
117-81-7	bis(2-ethylhexyl)phthalate		X		X	X	X
117-84-0	Di-n-octylphthalate		X			X	
118-74-1	Hexachlorobenzene (perchlorobenzene)	F024, F025, K016, K018, K030, K042, K085, K149, K150, K151	X		X	X	X
118-96-7	2,4,6-Trinitrotoluene		X				
119-90-4	3,3'-Dimethoxybenzidine		X			X	
119-93-7	3,3'-Dimethylbenzidine						
120-12-7	Anthracene	K022	X		X	X	
120-58-1	Isosafrole						
120-62-7	Piperonyl sulfoxide						
120-71-8	p-Cresidine						
120-80-9	Catechol						
120-82-1	1,2,4-Trichlorobenzene	F024, F025, K085, K150	X		X	X	X
120-83-2	2,4-Dichlorophenol	K043, K099	X		X	X	
121-14-2	2,4-Dinitrotoluene	K025, K111	X			X	

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US EPA ARCHIVE DOCUMENT

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121-44-8	Triethylamine	K156, K157					
121-69-7	N,N-Diethyl aniline						
121-75-5	Malathion		X				
122-09-8	a,a-Dimethylphenethylamine						
122-39-4	Diphenylamine	K083, K104	X			X	
122-66-7	1,2-Diphenylhydrazine		X			X	
123-31-9	Hydroquinone						
123-33-1	Maleic hydrazide		X			X	
123-38-6	Propionaldehyde					X	
123-63-7	Paraldehyde	K009, K010, K026					
123-91-1	Dioxane (1,4-dioxane)		X		X	X	
124-48-1	Chlorodibromomethane		X				X
126-68-1	0,0,0-Triethyl phosphorothioate						
126-72-7	tris(2,3-dibromopropyl) phosphate						
126-75-0	Demeton-S						
126-98-7	Methacrylonitrile		X			X	
126-99-8	Chloroprene						
127-18-4	Tetrachloroethene (Perchloroethylene)	F001, F002, F024, F025, K016, K019, K020, K073, K116, K150, K151	X		X	X	X
129-00-0	Pyrene	K022	X		X		X
130-15-4	1,4-Naphthoquinone	K024					
131-11-3	Dimethyl Phthalate		X		X	X	

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US EPA ARCHIVE DOCUMENT

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INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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131-89-5	2-Cyclohexyl-4,6-dinitro-phenol		X				
131-89-5	2-Cycloyhexyl-4,6-dinitrophenol					X	
132-32-1	3-Amino-9-ethylcarbazole						
132-64-9	Dibenzofuran				X		
133-06-2	Captan				X		
133-90-4	Chloramben						
134-32-7	1-Naphthylamine (alpha-naphthylamine)						
137-17-7	2,4,5-Trimethylaniline						
137-26-8	Thiram						
140-57-8	Aramite						
140-88-5	Ethyl acrylate						
141-66-2	Dicrotophos						
143-33-9	Sodium cyanide	F007, F008, F009, F010, F011					
143-50-0	Kepone						
145-73-3	Endothall		X			X	
148-82-3	Melphalan						
151-50-8	Potassium cyanide	F007, F008, F009, F010, F011					
151-56-4	Ethylene imine (Aziridine)						
152-16-9	Octamethyl pyrophosphoramide						
156-60-5	(trans)1,2-dichloroethene	F024, F025	X			X	
156-62-7	Calcium cyanamide						
189-55-9	Dibenzo(a,i)pyrene						

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US EPA ARCHIVE DOCUMENT

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191-24-2	Benzo(g,h,i)perylene	K022			X	X	
192-65-4	Dibenzo(a,e)pyrene						
192-97-2	Benzo(e)pyrene	K022				X	
193-39-5	Indeno(1,2,3-cd)pyrene	F032, F034, K001, K022, K035, K141, K142, K147, K148	X			X	
205-82-3	Benzo(j)fluoranthene	K022			X	X	
205-99-2	Benzo(b)fluoranthene (3,4-Benzofluoranthene)	K001, K022, K035, K141, K142, K143, K144, K147, K148	X		X	X	
206-44-0	Fluoranthene	K001, K022, K035	X		X	X	X
207-08-9	Benzo(k)fluoranthene	F034, K022, K141, K142, K143, K144, K147, K148	X		X	X	
208-96-8	Acenaphthalene	K001, K022, K035					
218-01-9	Chrysene	F037, F038, K001, K022, K035	X		X	X	
224-42-0	Dibenz(a,j)acridine						
225-51-4	Benz[c]acridine						
297-97-2	O,O-Diethyl O-pyrazinyl phosphorothioate						
297-97-2	Thionazine						
298-00-0	Methyl parathion		X				
298-02-2	Phorate	K038, K040	X				
298-03-3	Demeton-O						
298-04-4	Disulfoton		X				
299-84-3	Ronnel		X				
300-76-5	Naled		X				

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US EPA ARCHIVE DOCUMENT

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302-01-2	Hydrazine						
302-17-0	Chloral hydrate						
303-34-1	Lasiocarpine						
305-03-3	Chlorambucil						
309-00-2	Aldrin		X				
311-45-5	Diethyl-p-nitrophenyl phosphate						
315-18-4	Mexacarbate						
319-84-6	alpha-Hexachlorocyclohexane (alpha-BHC)	F024	X			X	
319-85-7	beta-Hexachlorocyclohexane (beta-BHC)		X			X	
319-86-8	delta-BHC						
321-60-8	2-Fluorobiphenyl						
334-88-3	Diazomethane						
353-50-4	Carbon oxyfluoride						
357-57-3	Brucine						
367-12-4	2-Fluorophenol						
460-00-4	4-Bromofluorobenzene						
460-19-5	Cyanogen (oxalonitrile)		X			X	
463-58-1	Carbonyl sulfide						
465-73-6	Isodrin						
470-90-6	Chlorfenvinphos						
479-45-8	Tetryl						
492-80-8	Auramine						

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US EPA ARCHIVE DOCUMENT

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494-03-1	Chlornaphazin						
504-24-5	4-Aminopyridine						
505-60-2	Mustard gas						
506-61-6	Potassium silver cyanide	F006, F007, F008, F009, F010, F011, F012, F019, K007, K088					
506-64-9	Silver cyanide	F006, F012, F019, K007, K088					
506-68-3	Cyanogen bromide (bromocyanide)		X			X	
506-77-4	Cyanogen chloride		X			X	
510-15-6	Chlorobenzilate		X			X	
512-56-1	Trimethyl phosphate						
528-29-0	1,2-Dinitrobenzene (o-Dinitrobenzene)		X			X	
532-27-4	2-Chloroacetophenone					X	
534-52-1	4,6-Dinitro-o-cresol	F004				X	
540-36-3	1,4-Difluorobenzene						
540-73-8	1,2-Dimethylhydrazine					X	
540-84-1	2,2,4-Trimethylpentane					X	
541-53-7	Dithiobiuret						
541-73-1	1,3-Dichlorobenzene	F024, F025, K085, K105				X	X
542-62-1	Barium cyanide						
542-75-6	1,3-Dichloropropene		X			X	
542-76-7	3-Chloropropionitrile						
542-88-1	bis(Chloromethyl)ether	K017	X		X	X	

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US EPA ARCHIVE DOCUMENT

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544-92-3	Copper cyanide						
557-19-7	Nickel cyanide						
557-21-1	Zinc cyanide						
563-12-2	Ethion						
563-68-8	Thallium(I)acetate						
584-84-9	2,4-Toluene diisocyanate	K027				X	
590-60-2	Bromoethene					X	
591-08-2	1-Acetyl-2-thiourea						
591-78-6	2-Hexanone (butyl methyl ketone)						
592-01-8	Calcium cyanide						
593-60-2	Vinyl bromide						
598-31-2	Bromoacetone						
602-87-9	5-Nitroacenaphthene						
606-20-2	2,6-Dinitrotoluene		X			X	
608-93-5	Pentachlorobenzene	F024, F025, K085, K149, K150, K151	X		X	X	X
615-53-2	N-Nitroso-N-methylurethane						
621-64-7	N-Nitroso-di-n-propylamine		X				
623-40-5	Toluene-2,6-diamine		X			X	
624-83-9	Methyl isocyanate					X	
628-86-4	Mercury fulminate						
630-10-4	Selenourea						
630-20-6	1,1,1,2-Tetrachloroethane	F024, F025, K019, K020, K030, K095	X		X	X	

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US EPA ARCHIVE DOCUMENT

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636-21-5	o-Toluidine hydrochloride						
640-19-7	Fluoroacetamide						
680-31-9	Hexamethylphosphoramide						
684-93-5	N-Nitroso-N-methylurea						
692-42-2	Diethylarsine						
696-28-6	Dichlorophenylarsine						
732-11-6	Phosmet						
755-04-5	Titanium tetrachloride						
757-58-4	Hexaethyl tetraphosphate						
759-73-9	N-Nitroso-N-ethylurea						
764-41-0	1,4-Dichloro-2-butene					X	
765-34-4	Glycidylaldehyde		X			X	
786-19-6	Carbophenothion						
822-06-0	Hexamethylene-1,5-diisocyanate					X	
924-16-3	N-Nitroso-di-n-Buetylamine		X			X	
930-55-2	N-Nitrosopyrrolidine						
959-98-8	Endosulfan I						
961-11-5	Tetrachlorvinphos						
1024-57-3	Heptachlor epoxide		X				
1031-07-8	Endosulfan sulfate						
1116-54-7	N-Nitrosodiethanolamine						
1120-71-4	1,3-Propane sultone					X	

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US EPA ARCHIVE DOCUMENT

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1303-28-2	Arsenic pentoxide						
1314-32-5	Thallic oxide						
1314-62-1	Vanadium pentoxide						
1319-77-3	Cresols/cresylic acid (isomers and mixtures)	F004					
1327-53-3	Arsenic trioxide						
1330-20-7	Xylene (total)		X		X		X
1332-21-4	Asbestos						
1335-32-6	Lead subacetate						
1336-36-3	Polychlorinated biphenyls (209 congeners)		X		X	X	X
1338-23-4	2-Butanone peroxide						
1464-53-5	1,2,3,4-Diepoxybutane						
1563-66-2	Carbofuran	K156, K158					
1582-09-8	Trifluralin						
1615-80-1	N,N'-Diethylhydrazine						
1634-04-4	Methyl tert butyl ether					X	
1718-51-0	Terphenyl-d14						
1746-01-6	2,3,7,8-Tetrachlorodibenzo(p)dioxin (TCDD)	F020, F022, F023, F026, F027, F028, F032	X		X	X	X
1836-75-5	Nitrofen						
1888-71-7	Hexachloropropene						
2037-26-5	Toluene-d8						
2104-64-5	EPN						

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US EPA ARCHIVE DOCUMENT

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2303-16-4	Diallate (cis or trans)						
2310-17-0	Phosalone						
2385-85-5	Mirex						
2425-06-1	Captafol						
2763-96-4	5-(Aminomethyl)-3-isoxazolol						
2921-88-5	Chlorpyrifos		X				
3114-55-4	Chlorobenzene-d5						
3288-58-2	O,O-Diethyl S-methyl dithiophosphate						
3689-24-5	Tetraethyl dithiopyrophosphate						
4170-30-3	Crotonaldehyde (Propylene aldehyde)		X			X	
4549-40-0	N-Nitrosomethylvinylamine						
5131-60-2	4-Chloro-1,3-phenylenediamine						
5344-82-1	1-(o-Chlorophenyl)thiourea						
6533-73-9	Thallium(I)carbonate						
6923-22-4	Monocrotophos						
6959-48-4	3-(Chloromethyl)pyridine hydrochloride						
7005-72-3	4-Chlorophenyl phenyl ether	F020, F023, F027, F028					
7421-93-4	Endrin aldehyde						
7439-92-1	Lead	F035, F037, F038, K002, K003, K005, K046, K048, K049, K051, K052, K061, K062, K064, K069, K086, K100	X		X	X	X
7439-96-5	Manganese				X		X
7439-97-6	Mercury	K071, K106	X		X	X	X

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US EPA ARCHIVE DOCUMENT

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7440-02-0	Nickel	F006	X		X	X	X
7440-22-4	Silver		X		X	X	
7440-28-0	Thallium		X		X	X	
7440-36-0	Antimony	K021, K161	X		X	X	
7440-38-2	Arsenic	F032, F034, F035, K031, K060, K084, K101, K102, K161	X		X	X	X
7440-39-3	Barium		X		X	X	
7440-41-7	Beryllium		X			X	X
7440-43-9	Cadmium	F006, K061, K064, K069, K100	X		X	X	X
7440-47-3	Chromium (total)	F032, F034, F035, F037, F038, K090			X	X	X
7440-48-4	Cobalt						
7440-50-8	Copper						X
7440-62-2	Vanadium						
7440-66-6	Zinc				X		X
7446-18-6	Thallium(I)sulfate						
7487-94-7	Mercuric chloride		X				
7488-56-4	Selenium sulfide						
7647-01-0	Hydrogen Chloride (hydrochloric acid)		X				X
7664-38-2	Phosphoric acid						
7664-39-3	Hydrogen fluoride						X
7664-41-7	Ammonia		X			X	X
7700-17-6	Crotoxyphos						

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US EPA ARCHIVE DOCUMENT

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INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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7723-14-0	Phosphorus						
7778-39-4	Arsenic acid						
7782-41-4	Fluorine						
7782-49-2	Selenium		X		X	X	
7782-50-5	Chlorine		X				
7783-00-8	Selenium dioxide						
7783-06-4	Hydrogen sulfide						
7786-34-7	Mevinphos						
7791-12-0	Thallium(I)chloride						
7803-51-2	Phosphine						
7803-55-6	Ammonium vanadate						
8001-35-2	Toxaphene (chlorinated camphene)	K041, K098					
8065-48-3	Demeton						
10102-43-9	Nitric oxide						
10102-44-0	Nitrogen dioxide						X
10102-45-1	Thallium(I)nitrate						
10595-95-6	N-Nitrosomethylethylamine						
11096-82-5	Arochlor-1260						
11097-69-1	Arochlor-1254		X				
11104-28-2	Arochlor-1221						
11141-16-5	Arochlor-1232						
12039-52-0	Thallium(I)selenite						

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US EPA ARCHIVE DOCUMENT

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INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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12672-29-6	Arochlor-1248						
12674-11-2	Arochlor-1016		X				
13071-79-9	Terbufos						
13171-21-6	Phosphamidon						
13463-39-3	Nickel carbonyl						
13765-19-0	Calcium chromate						
16752-77-5	Methomyl						
18540-29-9	Chromium (hexavalent)	F006, F019, K002, K003, K004, K005, K006, K007, K008, K048, K049, K050, K051, K061, K062, K069, K086, K100	X		X		X
18883-66-4	Streptozotocin						
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
20816-12-0	Osmium tetroxide						
20830-81-3	Daunomycin						
20859-73-8	Aluminum phosphide						
21609-90-5	Leptophos						
22967-92-6	Methyl mercury		X		X	X	
23950-58-5	Pronamide		X			X	
25013-15-4	Methyl styrene		X				
25265-76-3	Phenylenediamine	K083, K103, K104					
25376-45-8	Toluenediamine						
26471-62-5	Toluene diisocyanate						
33213-65-9	Endosulfan II						

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US EPA ARCHIVE DOCUMENT

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INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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33245-39-5	Fluchloralin						
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin	F032			X	X	
39196-18-4	Thiofanox						
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
39300-45-3	Dinocap						
40321-76-4	1,2,3,7,8-Pentachlorodibenzo(p)dioxin	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
53469-21-9	Arochlor-1242						
53494-70-5	Endrin ketone						
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	F032			X	X	
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
57653-85-7	1,2,3,6,7,8,-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	F032			X	X	
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X		
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
125322-32-9	2,3,7,8-Tetrachlorodibenzofuran	F020, F022, F023, F026, F027, F028, F032			X	X	X
--	Beryllium compounds						
--	Cadmium compounds						
--	Chlorocyclopentadiene				X	X	
--	N-Chlorodiisopropyl amine						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

US EPA ARCHIVE DOCUMENT

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
--	N-Chloroisopropyl amine						
--	Chromium compounds						
--	Creosote	K001, K035					
--	Cyanide compounds	F006, F007, F008, F009, F010, F011, F012, F019, K007, K060, K088					
--	O-Decyl hydroxylamine						
--	Dibenzo(a,e)fluoranthene	K022			X	X	
--	Dibenzo(a,h)fluoranthene	K022			X	X	
--	Dibutylchloramine						
--	3,3-Dichloroisopropyl ether						
--	Dichloropentadiene					X	
--	Dimethylnitrosamine					X	
--	Lead compounds						
--	Nicotine salts						
--	2-Nitrodiphenylamine						
--	Octachlorodibenzo(p)dioxin				X	X	
--	Octachlorodibenzofuran				X	X	
--	Phthalic acid esters						
--	Saccharin salts						
--	Sodium O-ethylmethylphosphonate Diisopropylamine						
--	Strychnine salts						
--	Thioamine						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

US EPA ARCHIVE DOCUMENT

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
--	O-decyl-hydroxylamine						
--	Acenaphthene-d10						
--	Antimony compounds						
--	Arsenic compounds (inorganic, including arsine)						
--	2-Chloro-1,3-butadiene	F024, F025					
--	Chrysene-d12						
--	Cobalt compounds						
--	Coke oven emissions						
--	Dibenz(a)anthracene	K001, K035					
--	1,4-Dichlorobenzene-d4						
--	Dichloroethylene	K073					
--	Dichloropropane	F024, F025					
--	Dichloropropanols	K017					
--	Dichloropropene	F024, F025					
--	Manganese compounds						
--	Mercury compounds						
--	Naphthalene-d8						
--	Nickel compounds						
--	Nitrobenzene-d5						
--	Perylene-d12						
--	Phenanthrene-d10						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

US EPA ARCHIVE DOCUMENT

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
--	Phenol-d6						
--	Phenolic compounds	K060					
--	Phosphorodithioic and phosphorothioic acid esters	K036, K037, K038, K039, K040					
--	2,3,7,8-substituted Polychlorinated dibenzo(p)dioxin congeners (2,3,7,8-PCDDs)						
--	2,3,7,8-substituted Polychlorinated dibenzofuran congeners (2,3,7,8-PCDFs)						
--	Selenium compounds						
--	Tetrachlorobenzene	F024, F025					
--	2,4,6-Tribromophenol						
--	Trichloropropane	K017					

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

APPENDIX A-1

COMPOUNDS OF POTENTIAL INTEREST

REFERENCES AND DISCUSSION

This discussion lists reference documents for each of the columns in Table A1-1 and briefly describes the quality of data associated with these references. This information is only presented for informational purposes to assist in planning data collection.

A1.1 COLUMN 1: CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The CAS number is a unique number assigned to each compound in the table. Compounds are listed by CAS number, in ascending order, to prevent problems with alphabetization procedures or differences in common nomenclature.

A1.2 COLUMN 2: COMPOUND NAME

The most common compound name is listed. Where appropriate, common synonyms are also listed to aid the user in identifying particular compounds.

A1.3 COLUMN 3: COMPOUNDS LISTED IN 40 CFR PART 261 APPENDIX VII OR VIII

Appendix VII of Title 40 Code of Federal Regulations (40 CFR) Part 261 identifies compounds for which specific hazardous wastes, from specific and nonspecific sources, are listed (U.S. EPA 1995). Appendix VIII of 40 CFR Part 261 identifies acute hazardous wastes and toxic hazardous wastes associated with commercial chemical products, manufacturing chemical intermediates, and off-specification commercial chemical products (U.S. EPA 1995). This column lists hazardous waste codes for the associated compounds. This list is provided for reference purposes only, because it is commonly cited by other U.S. EPA combustion risk assessment documents as an original source of the product of incomplete combustion (PIC) lists. An explanation of the reasons for including a COPC on this list is beyond the scope of this guidance.

A1.4 COLUMN 4: CHEMICAL-SPECIFIC DATA AVAILABLE

This column lists those compounds for which the following are available (as presented in Appendix A-2): (1) chemical-specific physical and chemical information, and (2) chemical-specific fate-and-transport information.

A1.5 COLUMN 5: PICS RECOMMENDED BY U.S. EPA (1994a) FOR SCREENING LEVEL RISK ASSESSMENTS

Compounds in this column marked with an "X" in the appropriate cells identified by U.S. EPA (1994a) as PICs to be included in screening level risk assessments. U.S. EPA (1994a) does not describe the basis or references for the inclusion of these PICs in screening level risk assessments. More information regarding some of these compounds is presented in Chapter 2.

US EPA ARCHIVE DOCUMENT

A1.6 COLUMN 6: PICS IDENTIFIED IN COMBUSTION UNIT EMISSIONS (U.S. EPA 1993)

Compounds in this column marked with an "X" in the appropriate cells are identified in U.S. EPA (1993) as PICs. The source documents for these tables cited by U.S. EPA (1993) are described in the following subsections. These references have been cited by this and other U.S. EPA reference documents as "sources" of information regarding PIC emissions from hazardous waste combustion units. This document—U.S. EPA (1993)—has, in turn, been cited by later guidance documents as a "source" of information regarding PIC emissions from hazardous waste combustion units. However, as is indicated by the listing of the references from Dempsey and Oppelt (1993) (which is a summary of existing information), many of the reference documents appear to simply cite additional "sources" of information. The original research and sampling data regarding PIC emissions have not yet been identified but, based on a preliminary review of the information below, the sources of the "original" information cited by all of the most common reference documents may be limited and may have been published over 15 years ago.

A1.6.1 Demsey and Oppelt (1993)

The sections of Demsey and Oppelt (1993) regarding PICs from hazardous waste combustion facilities ("Combustion Byproduct Emissions" and "Table XVII: Organics that Could Potentially be Emitted from Devices Burning Hazardous Waste") cite the following references:

- U.S. EPA (1989b) does not include a list of PICs from combustion sources. U.S. EPA (1989b) discussed ways of ensuring that PIC emissions do not pose an unacceptable risk to human health and the environment. Stack gas carbon monoxide (CO) concentration is a good indicator of combustion efficiency; therefore, controlling CO is a prudent and reasonable approach to minimizing the potential risk from PICs. The destruction and removal efficiency (DRE) standard of 40 CFR Part 264.242(a) limits stack emissions of principal organic hazardous constituents (POHC) to 0.01 percent (or 0.0001 percent for dioxin-containing waste) of the quantity of POHC in the waste. This standard, however, does not impose a limit on PICs. Therefore, a limit of 100 parts per million by volume (ppmv) (Tier I) was imposed, below which PIC emissions do not pose unacceptable risks to human health. The proposed rule allows a waiver to the 100-ppmv CO limit, by (1) restricting total hydrocarbon (THC) emissions to 20 ppmv (Tier II), or (2) showing that THC emissions do not pose an unacceptable risk by using prescribed risk assessment procedures.

  The above limitations were also provided in the Federal Register, dated January 23, 1981 (U.S. EPA 1981) and April 27, 1990 (U.S. EPA 1990b)

- U.S. EPA (1981) does not contain any information regarding PICs not contained in U.S. EPA (1989b). There is no discussion of "risk" in this document. Although the notice deals with permitting standards, there is no risk-based approach, and it appears to be an entirely technical discussion. Specifically, it deals with updated material for specific parts of 40 CFR.

  - 40 CFR Part 122 (Incinerator Facility Permits)
  - 40 CFR Part 264 (General Standards for Hazardous Waste Incineration)
  - 40 CFR Part 265 (Interim Status Standards for Hazardous Waste Incineration)

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Standards are technology-based, not risk-based.

- U.S. EPA (1990a) describes amendments to the hazardous waste incinerator regulations for the following purpose:

> Improve control of toxic metal emissions, HCl emissions, and residual organic emissions; amend the definitions of incinerators and industrial furnaces; propose definitions for plasma arc incinerators and infrared incinerators; propose to regulate carbon regeneration units as thermal treatment devices; and make a number of minor revisions to permitting procedures.

U.S. EPA (1990a) also states the following:

> The database on PIC emissions is limited therefore, the risk assessments may under-estimate risk. The assessments consider only the organic compounds that have been actually identified and quantified. Zero to 60 percent of total unburned hydrocarbon emissions have been chemically identified at any particular facility. Thus, the bulk of the hydrocarbon emissions have not been considered in those risk assessments. Although many of the unidentified, unquantified organic compounds may be non-toxic, some fraction of the organic emissions is undoubtedly toxic. . . .data on typical PIC emissions from hazardous waste combustion sources were compiled and assessed in recent EPA studies. These studies identified 37 individual compounds in the stack gas of the eight full-scale hazardous waste incinerators tested, out of which 17 were volatile compounds and 20 semivolatile compounds. Eight volatile compounds (benzene, toluene, chloroform, trichloroethylene, carbon tetrachloride, tetrachloroethylene, chlorobenzene, and methylene chloride), and one semivolatile compound (naphthalene) were identified most frequently in more than 50 percent of the tests. Some of these compounds are carcinogenic.

The sources for these statements appear to be Wallace and others (1986) and Trenholm and Lee (1986).

Trenolm and Lee (1986), prepared by Andrew R. Trenholm of Midwest Research Institute and C.C. Lee at the U.S. EPA Hazardous Waste Engineering Research Laboratory, discussed that emissions from incinerators are only characterized for constituents listed in Appendix VIII. However, constituents not listed in Appendix VIII are also emitted from the stacks.

Data was obtained from HWERL-sponsored tests at eight hazardous waste incinerators, nine boilers that co-fired hazardous wastes, and five mineral processing kilns that fired hazardous wastes as fuel. In addition, SVOC emissions data for two municipal solid waste incinerators and seven coal-fired power plants were also reviewed. The common PICs are presented in the following table:

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Volatile PICs Most Frequently Present in Stack Gases	
VOCs	**SVOCs**
Benzene	Naphthalene
Toluene	Phenol
Carbon Tetrachloride	Bis(2-ethylhexyl)phthalate
Chloroform	Diethylphthalate
Methylene Chloride	Butylbenzylphthalate
Trichloroethylene	Dibutylphathlate
Tetrachloroethylene	
1,1,1-Trichloroethane	
Chlorobenzene	

Tests were conducted for three incinerator runs to search for constituents not listed in Appendix VIII . These constituents include:

Non-Appendix VIII Constituents Present in Highest Concentrations in Stack Gases	
Acetone	Ethylbenzaldehyde
Ethylbenzene	Ethylbenzoic acid
Acetophenone	Ethylphenol
Benzaldehyde	Ethylphenyl-ethanone
Benzenedicarboxaldehyde	Ethynylbenzene
Benzoic acid	Phenylacetylene
Chlorocyclohexanol	1,1'-(1,4-phenylene)bisethanone
Cyclohexane	Phenylpropenol
Cyclohexanol	Propenylmethylbenzene
Cyclohexene	Tetramethyloxirane
Dioctyl adipate	Trimethylhexane
Ethenyl ethylbenzene	

Emission rates of compounds not in the waste feed were also provided.

- U.S. EPA (1985) does not include a list of PICs from combustion sources. U.S. EPA (1985) discussed views and reviews by the Environmental Effects, Transport, and Fate Committee of the Science Advisory Board of issues related to the environmental impacts of the incineration of liquid hazardous wastes at sea and on land. Several issues were

US EPA ARCHIVE DOCUMENT

addressed, including issues concerning the combustion and incineration of hazardous waste. Major findings of the committee were as follows:

- Fugitive emissions and spills may release as much or more material to the environment than the direct emissions from waste incineration processes.

- Numerous PICs are formed during combustion processes. However, only a fraction of them are identified or detected. It is possible that the aggregate of all compound emissions that are not categorized as other POHCs or PICs can be more toxic and pose greater risks than those listed. Although 99.99 percent DRE has been claimed, if the unburned or undetected hydrocarbon output is included, the DRE may actually be less than 99.99 percent. Therefore, the concept of destruction efficiency used by EPA was found to be incomplete and not useful for subsequent exposure assessments. All emissions and effluents must be identified and quantified, including their physical form and characteristics.

- Local site-specific conditions must be used in characterizing exposure to receptors from waste incinerator emissions.

- The evaluation of exposure durations and concentrations should be based on a detailed assessment of transport processes and the habits of the exposed organisms. The role of food chains needs particular attention.

- At a minimum, the toxicities of representative emissions and effluents from incinerators should be tested on sensitive life stages of representative aquatic and terrestrial vertebrates, invertebrates, and plants of ecological importance.

• U.S. EPA (1990b) does not include a list of PICs from combustion sources. It was prepared by the PIC subcommittee of the Science Advisory Board to review the OSW proposal to control emissions of PICs from hazardous waste incinerators by instituting process controls that are based on CO and THC emission concentrations. U.S. EPA risk assessments indicate that emissions of PICs at currently measured levels are not likely to produce unacceptable risks. However, because the current DRE standard applies only to designated POHCs, 99.99 percent DRE does not preclude the possibility that emission of PICs could present significant risk. The following summarizes the major findings of the subcommittee review.

- The concept of using CO and THC as guidance for incinerator operational control is reasonable.

- At low CO levels, CO correlates well with THC; therefore, limiting CO in order to ensure high combustion efficiency and low THC levels is reasonable. At high CO concentrations, CO and THC do not correlate well; therefore, relying solely on the controlling of CO may not provide a reasonable control for THC. Continuous emissions monitoring of THC is preferred. Quantification of PICs alone is not practical with the sampling techniques that are available, primarily because PICs are normally emitted in the range of parts per billion (ppb) to parts per trillion (ppt).

US EPA ARCHIVE DOCUMENT

- A 100-ppmv limit for CO is reasonable. However, supporting documentation does not demonstrate that a CO concentration of 100 ppmv is better than 50 ppmv or 150 ppmv.

- Continuous emissions monitoring of THC with a cold system appears to be practical for routine operations. However, a hot transfer line produces better analysis of THC concentrations and detection of a larger fraction of the THCs emitted.

- The database characterizing PICs in emissions would not allow a correlation to be established with CO or THC levels for various combustion devices and conditions. Limited data introduces large uncertainties into U.S. EPA's risk assessment. Therefore, U.S. EPA's site-specific risk assessment process is limited in its usefulness in establishing acceptable THC levels. However, the risk assessment procedures are risk-based.

• U.S. EPA (1987) is a report prepared by Andrew R. Trenholm, Acurex Corporation, California, and staff members from the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. The paper discussed the lack of information on total emissions from combustion of hazardous wastes, particularly under conditions of less than optimal performance. The focus issue was whether additional constituents that are listed in Appendix VIII or not listed in Appendix VIII which were not identified in early tests might be emitted from hazardous waste combustion units. To address this issue and related issues, U.S. EPA initiated this project to qualitatively and quantitatively study the characteristics of all possible effluents, under steady-state and transient conditions. The following summarizes the major findings:

  - THC emissions detected as specific compounds ranged from 50 to 67 percent for five runs and were 91 percent for one run. The fraction of THC not detected is most likely explained by uncertainty in the measurements or other analytical problems.

  - Methane accounted for the largest fraction of THC.

  - Oxygenated aliphatic compounds made up the largest class of compounds among the SVOCs, both in total mass and number of compounds.

  - Transient upsets did not cause significant increases in the concentration of SVOCs or most VOCs. Three VOCs that were increased were methane, methylene chloride, and benzene.

  - Particulate and HCl emissions did not change between the steady-state and transient test runs.

• Duval and Rubey (1976) was prepared by D.S. Duval and W.A. Rubey of the University of Dayton Research Institute, Ohio. The objective of the study was to provide data from which requirements can be assigned for the thermal disposal of kepone. This report was primarily concerned with the high-temperature destruction of kepone, with DDT and Mirex used as comparative Analog. Laboratory tests were conducted to establish

US EPA ARCHIVE DOCUMENT

destruction temperature characteristics of the vaporized pesticides at preselected residence times. The following summarizes the major findings.

- Kepone was essentially destroyed at a 1-second residence time and a temperature range of 500°C to 700°C, depending on the pesticide.

- Major decomposition products detected were hexachlorocyclopentadiene and hexachlorobenzene for both kepone and Mirex. These products were formed in different thermal regions.

- The study demonstrated that the chemical nature of the effluent products depends on the temperature and residence time that the basic molecule experiences.

- Duval and Rubey (1977) discusses the experimental destruction temperature and residence time relationships for various PCB compounds and mixtures of PCBs. The document states that "upon thermal stressing in air, PCBs decomposes to low-molecular-weight products." However, the document does not identify any of these low-molecular-weight products. In fact, the document states directly that the products were not identified in the study. It further recommends that additional research be conducted on the "degradation products and effluents."

- Dellinger, Torres, Rubey, Hall, and Graham (1984) was prepared by Barry Dellinger and others of the University of Dayton, Ohio. This paper presented the gas-phase thermal stability method under controlled laboratory conditions to rank the incinerability of compounds. The objective of this study was to determine the gas-phase thermal decomposition properties of 20 hazardous organic compounds.

  The compounds were selected on the basis of (1) frequency of occurrence in hazardous waste samples, (2) apparent prevalence in stack effluents, and (3) representativeness of the spectrum of hazardous waste organic waste materials. The following summarizes the major findings.

  - Gas-phase thermal stability method is a more effective means of ranking the incinerability of hazardous compounds in a waste.

  - Numerous PICs were formed during the thermal decomposition of most of the compounds tested. However, PICs were not identified.

  - Destruction efficiency of 99.99 percent is achieved at 2 seconds mean residence time in flowing air at 600°C to 950 °C.

  - No single physical or chemical property describes the ranking scheme for incinerability.

- Dellinger, Hall, Graham, Mazer, Rubey, and Malanchuk (1986) was prepared by Barry Dellinger, B. Douglas, L. Hall, John L. Graham, Sueann L. Mazer, and Wayne A. Rubey of the University of Dayton Research Institute, Dayton, Ohio, and Myron Malanchuk of U.S. EPA, Cincinnati, Ohio. The paper discussed the development of an incineration

US EPA ARCHIVE DOCUMENT

model based on laboratory studies conducted by using the nonflame mode of hazardous waste thermal decomposition. The results of these studies were compared to the flame-mode studies and field tests to evaluate the incineration model proposed. The model was based on the premise that incinerators do not operate continuously at optimum conditions. As a result, 1 percent or more of the feed and its flame treatment products must undergo further decomposition in the nonflame region to meet the DRE criterion of greater than 99.99 percent.

In the past, several methods were used to rank the incinerability of compounds. Nonflame studies, however, indicated that tests on compounds conducted at low oxygen concentrations provided a better correlation with field tests to determine the relative incinerability of compounds. Four experimental studies were conducted to develop and expand the database on POHCs and PICs.

Studies were conducted on individual compounds to evaluate degradation compounds and PICs from the original parent compound. The thermal degradation of 2,3',4,4',5-PCB was studied under four reaction atmospheres (at varying levels of oxygen) at a constant gas phase residence time of 2.0 seconds. Tests were conducted at temperatures ranging from 500°C to 1,000°C. Tests indicated that the yield of combustion products decreased with increased oxygen levels. Numerous major degradation products were identified from the thermal degradation of 2,3',4,4',5-PCB, including:

- Penta-, tetra-, and trichlorodibenzofurans
- Tetra- and trichlorobiphenyls
- Tri- and dichlorobenzene
- Tetra- and trichloronaphthalene
- Tri- and dichlorochlorophenylethlyene
- Tetrachlorobiphenylenes
- C_9H_8OCl
- $C_{10}H_3Cl_3$

Thermal decomposition of chloroform was studied. Numerous decomposition products were identified, including:

- CCl_4
- $C_2H_4Cl_2$
- C_2HCl_3
- C_2HCl_5
- C_2Cl_2
- C_2Cl_4
- C_3Cl_4
- C_4Cl_6

Thermal decomposition of polychlorinated phenols was studied in nitrogen (N_2) and oxygen atmospheres because of the potential formation of polychlorinated dibenzodioxins. Pentachlorophenol (PCP) thermal decomposition was studied. Numerous decomposition products of PCP were identified in N_2 and/or air atmospheres, including:

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- Dichlorobutadiyne (in N_2)
- Tetrachloroethylene (in air)
- Tetrachloropropyne (in air)
- Trichlorofuran (in air)
- Tetrachlorofuran (in air)
- Trichlorobenzene (in N_2 and air)
- Tetrachlorobenzene (in N_2 and air)
- Pentachlorobenzene (in N_2 and air)
- Hexachlorobenzene (in N_2)
- Octachlorostyrene (in N_2)
- Hexachlorodihydronaphthalene (in N_2 and air)

The paper concluded that PICs in the air atmosphere may have formed directly from the parent material, whereas, in the nitrogen atmosphere, the principal PICs may have evolved from the thermal decomposition of other PICs.

- Kramlich, Seeker, and Heap (1984) does not include a list of PICs from combustion sources. It was prepared by J.C. Kramlich, W.R. Seeker, and M.P. Heap of Energy and Environmental Research Corporation, California; and C.C. Lee of the Industrial Waste Combustion Group, U.S. EPA. This paper presented a research program to study the flame-mode incineration of hazardous waste liquids in laboratory scale reactors. The objective of this study was to supply the flame-mode data that will be used in evaluating the applicability of various approaches to ranking the ease of incinerability.

  Five compounds were tested—chloroform, 1,1-dichloroethane, benzene, acrylonitrile, and chlorobenzene—because (1) their range of incinerabilities is broad, and (2) they are representative of liquid hazardous wastes. The following summarizes the findings.

  - The flame section of the incinerator destroys greater than 99.995 percent of the wastes.
  - The post-flame region destroys the remainder of the wastes.
  - The destruction efficiency is reduced because of flame-related failures.
  - Incinerability ranking depends on actual failure condition.
  - No incinerability ranking system completely predicts the destruction efficiency of the compounds tested for all failure conditions.

- Trenholm and Hathaway (1984) was prepared by Andrew Trenholm and Roger Hathaway of Midwest Research Institute (MRI) in Missouri, and Don Oberacker, U.S. EPA, Cincinnati, Ohio. PICs were defined as any Appendix VIII hazardous organic constituent detected in the stack gas but not present in the waste feed at a concentration of 100 micrograms per gram or higher. Benzene and chloroform were the most commonly found PICs. PIC emissions were comparable to POHC emissions in concentration and total mass output. This document discussed PIC formation mechanisms and criteria for PIC formations.

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MRI conducted a series of tests at eight operating hazardous waste incineration facilities and analyzed the collected samples for PICs. These tests were conducted as part of the technical support of U.S. EPA's preparation of a regulatory impact analysis for hazardous waste incinerators. Each incinerator had a liquid injection burner, and some facilities also included a rotary kiln or hearth. Three incinerators had no air pollution control devices. The remaining five had wet scrubbers for HCl control, and four of these had other particulate control devices. Twenty-nine compounds were classified as PICs from the eight incinerator tests and are presented in Table A1.6-1. In general, PIC concentrations were slightly higher than POHC concentrations, although this ratio varied from site to site. PIC output rate very rarely exceeded 0.01 percent of the POHC input rate. The document stated that the measurement of Appendix VIII compounds at low concentrations in the waste feed, auxiliary fuel, and inflow streams to control systems is often necessary to explain the presence of PICs.

- Olexsey, Huffman, and Evans (1985) was prepared by Robert A. Olexsey and others of the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. This document discussed PIC generation mechanisms and criteria for PIC formations. The paper provided data on emissions of PICs during full-scale tests conducted on incinerators and boilers burning hazardous waste (Trenholm and others 1984; Castaldini and others 1984). The documents referenced by this paper summarized a series of full-scale tests conducted on seven incinerators and five boilers conducted by U.S. EPA to support its regulatory development for incinerators and boilers. Commonly found PICs identified in these tests are presented in Tables A1.6-2 and A1.6-3.

- For incinerators, ratios of PIC emissions to POHC input ranged from 0.00007 to 0.0028 percent; and ratios of PIC emissions to POHC emissions ranged from 0.01 to 3.89. For boilers, ratios of PIC emissions to POHC input ranged from 0.0032 to 0.3987 percent, and ratios of PIC emissions to POHC emissions ranged from 5.44 to 22.5. These data indicated that PIC emissions were higher for boilers than for incinerators; that is, PIC emissions were reduced with increased POHC DRE which is higher for incinerators. The document proposed seven methods to control PICs and recommended further research on PIC generation mechanisms and control technologies.
- Trenholm, Kapella, and Hinshaw (1992) was prepared by Andrew R. Trenholm and David W. Kapella of MRI in North Carolina and Gary D. Hinshaw of MRI in Missouri. The paper discusses the following issues regarding emissions from incinerators that burn hazardous waste: (1) emissions of specific constituents presented in Appendix VIII, (2) emissions of specific compounds or types of compounds, and (3) data on the size and molecular weight of compounds emitted. The following were among the major issues discussed.

    - PICs were studied through U.S. EPA-sponsored tests at eight incinerators, nine industrial boilers, and five mineral processing kilns. The study was limited to compounds presented in Appendix VIII. In all, 52 organic compounds (32 VOCs and 20 SVOCs) were identified. The VOC concentrations were significantly higher than the SVOC concentrations. PICs listed in this paper included benzene, toluene, carbon tetrachloride, trichloromethane, dichloromethane, trichloroethene, tetrachloroethene, 1,1,1-trichloroethane, cholorobenzene, naphthalene, and phenol.

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TABLE A1.6-1

PICS IDENTIFIED BY TRENHOLM AND HATHAWAY (1984)

PICs Found In Stack Effluents			
PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Bromodichloromethane	4	3	32
Dibromochloromethane	4	1	12
Naphthalene	3	5	100
Bromoform	3	0.2	24
Chlorobenzene	3	1	10
Tetrachloroethylene	3	0.1	2.5
1,1,1,-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
o-Nitrophenol	2	2	50
Methylene chloride	2	2	27
Phenol	2	4	22
2,4,6-Trichlorophenol	1	110	110
Carbon disulfide	1	32	32
o-Chlorophenol	1	22	22
2,4-Dimethylphenol	1	21	21
Methylene bromide	1	18	18
Bromochloromethane	1	14	14
Trichlorobenzene	1	7	7
Hexachlorobenzene	1	7	7
Diethyl phthalate	1	7	7
Pentachlorophenol	1	6	6
Dichlorobenzene	1	4	4
Chloromethane	1	3	3
Methyl ethyl ketone	1	3	3
Bromomethane	1	1	1
Pyrene	1	1	1
Fluoranthene	1	1	1

Notes:

ng/L = Nanograms per liter
PIC = Product of incomplete combustion

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TABLE A1.6-2

VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN BOILER EMISSIONS (OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Chloroform	5	4.2	1,900
Tetrachloroethylene	5	0.3	760
Chloromethane	4	4.6	410
Methylene chloride	4	83	2,000
Benzene	3	9.4	270
1,1,1-Trichloroethane	3	5.9	270
1,2-Dichloroethane	3	1.3	1,200

Notes:
ng/L = Nanograms per liter
PIC = Product of incomplete combustion

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TABLE A1.6-3

VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN INCINERATOR EMISSIONS (OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Tetrachloroethylene	3	0.1	2.5
1,1,1-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
Methylene chloride	2	2	27

Notes:

ng/L = Nanograms per liter
PIC = Product of incomplete combustion

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- From the U.S. EPA-sponsored tests, (1) volatile compounds listed in Appendix VIII identified were only a fraction—sometimes about one-half—of the total organic compounds identified, and (2) semivolatile compounds not listed in Appendix VIII identified were three to 30 times the quantity of organic compounds listed in Appendix VIII . Table A1.6-4 lists the compounds identified by the U.S. EPA-sponsored tests.

- A study of hazardous waste incinerator stack effluent was conducted to characterize the types of compounds emitted. Twenty-nine compounds were identified at a concentration range of 0.1 to 980 nanograms per liter. Methane, chloromethane, and chloroform accounted for more than one-half of the total mass of VOCs detected. Other than methane, oxygenated aliphatic hydrocarbons formed the highest fraction of the total emissions.

- Based on the incinerator stack effluent study, it was found that as combustion conditions deteriorate, increases in mass emissions are first noted with VOCs. Emissions of these compounds, most notably C1 to C3 compounds, increase proportionately more than larger compounds. For larger compounds, available data indicate that emission increases are more likely to be aromatic compounds.

A1.6.3 CARB (1990b)

CARB prepared "Technical Support Document of Proposed Dioxins Control Measures for Medical Waste Incinerators" to meet the requirements of California Health and Safety Code Section 39666 that a needs report be prepared for proposed rules. The report presents a proposed airborne toxic control measure for dioxin emissions from medical waste-burning facilities. The report concentrates on dioxin, furan, and cadmium emissions, although other pollutants detected during the tests are listed. Table A1.6-5 lists these pollutants.

A1.6.4 CARB (1991)

CARB prepared "Air Pollution Control at Resource Recovery Facilities 1991 Update" to update information presented in its 1984 report, entitled "Air Pollution Control at Resource Recovery Facilities." Specifically, the document updates available guidelines concerning incinerator technology, emissions control technology, and emission limits for municipal waste, hospital waste, biomass, tire, manure, landfill and digester gas, and sewer sludge incinerators. The document states that its guidelines represent levels that have been achieved by existing facilities.

In addition, the document summarizes the ultimate analysis of waste types undergoing treatment in the facilities described above. An appendix summarizes stack gas analysis data for numerous operating facilities. Pollutants identified in the analyses are summarized in Table A1.6-6.

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TABLE A1.6-4

MOST FREQUENTLY IDENTIFIED PICS (TRENHOLM, KAPELLA, AND HINSHAW 1992)

Appendix VIII Volatile Organic Compounds	Appendix VIII Semivolatile Organic Compounds	Compounds Not Listed in Appendix VIII
1,1,1-Trichloroethane	Bis(2-Ethylhexyl)phthalate	1,1'-(1,4-Phenylene)bisethanone
Benzene	Butylbenzylphthalate	Acetone
Carbon tetrachloride	Dibutylphtahlate	Acetophenone
Chlorobenzene	Diethylphthalate	Benzaldehyde
Chloroform	Naphthalene	Benzenedicarboxaldehyde
Methylene chloride	Phenol	Benzoic acid
Tetrachloroethylene		Cyclohexanol
Toluene		Chlorocyclohexanol
Trichloroethylene		Cyclohexane
		Ethylbenzene
		Ethylbenzoic acid
		Ethylphenol
		Ethylphenyl-ethanone
		Ethynylbenzene
		Phenylpropenol
		Propenylmethylbenzene
		Tetramethyloxirane
		Trimethylhexane

US EPA ARCHIVE DOCUMENT

TABLE A1.6-5

COPCS IDENTIFIED BY CARB (1990b)

COPC		
Ammonia	1,2-Dibromoethane	Nickel
Arsenic	Dichloroethane	Nitrogen oxides
Benzene	Dichloromethane	PM
Bromodichloromethane	1,2-Dichloropropane	PAHs
Cadmium	Ethylbenzene	Sulfur dioxide
Carbon dioxide	Freon	Tetrachloroethene
Carbon monoxide	Hydrocarbon, total	Tetratrichloromethylene
Carbon tetrachloride	Hydrogen chloride	Toluene
Chlorobenzenes	Hydrogen fluoride	Tribromomethane
Chlorodibromomethane	Iron	Trichlorethane
Chloroform	Lead	1,1,1-Trichloroethane
Chlorophenols	Manganese	Trichloroethylene
Chromium, hexavalent	Mercury	Trichlorotrifluroethane
Chromium, total	Mesitylene	Vinyl chloride
Copper	Methyl isobutyl ketone	Xylenes
Cumene	Napthalene	Zinc

Notes:

PAH = Polynuclear aromatic hydrocarbons
PM = Particulate matter

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TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

(Page 1 of 2)

Pollutant	Incinerator Type [a]						
	Municipal Waste (5)	Hospital Waste (7)	Biomass (4)	Manure (1)	Tire (1)	Landfill Gas (20)	Sewage Sludge and Digester Gas (5)
Nitrogen oxides	✔	✔	✔	✔	✔	✔	✔
Sulfur oxides	✔	✔	ND	✔	✔	✔	✔
Particulate matter	✔	✔	✔	✔	✔	✔	✔
Carbon monoxide	✔	✔	✔	✔	✔	✔	✔
Total hydrocarbons	✔	✔	✔	✔	✔	✔	✔
Hydrogen chloride	✔	✔	NA	NA	✔	NA	NA
Hydrogen fluoride	✔	NA	NA	NA	NA	NA	NA
Amonnia	NA	NA	✔	NA	✔	NA	NA
Carbon dioxide	✔	✔	✔	✔	✔	NA	✔
Oxygen	✔	✔	✔	✔	✔	NA	✔
Arsenic	✔	✔	✔	NA	✔	✔	✔
Beryllium	✔	NA	NA	NA	✔	✔ [b]	✔
Cadmium	✔	✔	✔	NA	ND	✔ [b]	✔
Chromium (total)	✔	✔	✔	NA	✔	✔	✔
Chromium (hexavalent)	ND	✔	NA	NA	✔	NA	NA
Copper	✔	NA	NA	NA	NA	✔	NA
Mercury	✔	✔	NA	NA	ND	✔	✔
Iron	NA	NA	✔	NA	NA	NA	NA
Manganese	NA	NA	✔	NA	NA	NA	NA
Nickel	✔	✔	✔	NA	ND	✔	✔
Lead	✔	✔	✔	NA	ND	✔	✔
Zinc	NA	NA	NA	NA	NA	✔	NA
Polyaromatic hydrocarbons [b]	✔	NA	✔	NA	✔	NA	NA
Polychlorinated biphenyls [b]	✔	ND	✔	NA	✔	NA	NA
CP [b]	✔	NA	✔	NA	✔	NA	NA
CB [b]	✔	NA	✔	NA	✔	NA	NA
Benzene	✔	✔	✔	NA	NA	NA	NA
Polychlorinated dibenzo(p) dioxins [b]	✔	✔	✔	NA	✔	NA	NA
Polychlorinated dibenzofurans [b]	✔	✔	✔	NA	✔	NA	NA
2,3,7,8-Tetrachloro dibenzo(p)dioxin equivalents [b]	✔	✔	✔	NA	✔	NA	✔

US EPA ARCHIVE DOCUMENT

TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

(Page 2 of 2)

Notes:

✔	=	Detected in at least one emission test
ND	=	Not detected in any emission test
NA	=	No analysis

[a] Number in parentheses indicates the number of facilities for which data were tabulated.

[b] Isomers and/or homologues that were not detected were added to total values at one-half the detection limit; pollutant may not have actually been detected.

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A1.6.5 U.S. EPA (1988)

This document, referenced by some documents as a 1989 document, was prepared in 1988.

U.S. EPA prepared "Hospital Waste Combustion Study: Data Gathering Phase" to assemble available information on hospital waste combustion so that U.S. EPA can evaluate whether airborne pollutant emissions from hospital waste combustion should be regulated. While preparing this document, U.S. EPA reviewed the pertinent literature to determine which studies would be helpful in completing the database on toxic emissions from medical waste incinerators. The report clearly addresses only those pollutants for which emissions data were found. The data reviewed were mostly for larger, controlled air incinerators; and the more commonly used retort incinerators were not evaluated.

The study identified several categories of pollutants that were measured in stack gases; these are discussed in the following paragraphs.

Where evaluated, acid gases were detected in stack gases. For example, HCl was detected in 24 of 28 tests; HCl concentration not recorded in the remaining four tests.

Particulate matter (PM) was detected in all stack tests for 30 facilities at concentrations ranging from 0.001 grains per dry standard cubic foot (gr/dscf), at a facility with PM add-on control devices, to 0.22 gr/dscf at facilities without such control devices.

Trace metals were detected in stack tests for three medical waste incineration facilities. Metals detected include arsenic, cadmium, chromium, iron, manganese, nickel, and lead. The document also states that fine-particle enrichment processes could lead to emissions of molybdenum, tin, selenium, vanadium, and zinc. However, test results for these trace metals are not presented.

With respect to organic emissions, dioxins and furans were detected in emissions from three facilities, both with and without pollution control devices. Other organic emissions detected in stack tests cited in this report include CO, THC, trichlorotrifluoroethane, tetrachloromethane, tetrachloroethene, and trichloroethylene.

In a stack testing conducted on three Canadian biomedical waste incinerators, PCBs and PAHs were either not detected (one facility) or not analyzed (two facilities).

A1.6.6 CARB (1996)

In May 1996, CARB prepared "Proposed Amendments to the Emission Inventory Criteria and Guidelines Report Published in Accordance with the Air Toxics 'Hot Spots' Information and Assessment Act of 1987." The purpose of the report is to present the basis of CARB's recommended amendments to the Air Toxics Hot Spots Program. The report states that California Health and Safety Code (HSC) 44321 requires CARB to compile the list of toxic substances that must be monitored from "designated reference lists of substances." Therefore, the document is not a primary source of toxics emission information. The primary sources of information are mandated by California HSC 44321, as follows:

- California HSC 44321(a): National Toxicology Program, International Agency for Research on Cancer
- California HSC 44321(b): Governor's List of Carcinogens and Reproductive Toxicants

US EPA ARCHIVE DOCUMENT

- California HSC 44321(c): CARB
- California HSC 44321(d): Hazard Evaluation System and Information Service
- California HSC 44321(e): U.S. EPA
- California HSC 44321(f): California HSC

The lists of toxic substances presented in the document are not restricted to incinerator facilities, but apply to any facility discharging airborne pollutants to the atmosphere. The document also removes numerous substances, primarily medicinal compounds, from lists of toxic chemicals that must always be evaluated, and places them on lists of toxic compounds that require evaluation only if a facility manufactures that substance.

A1.7 COLUMN 7: U.S. EPA-RECOMMENDED AND POTENTIAL PICS (1994a; 1994b)

Compounds marked with an "X" in the appropriate cells are identified in U.S. EPA (1994a and 1994b). Based on information presented in U.S. EPA (1994b), these tables were developed from available U.S. EPA data and from lists of toxic compounds from various U.S. EPA programs. Because the source lists were not developed as lists of toxic PICs, U.S. EPA deleted compounds that were not appropriate (U.S. EPA 1994b). U.S. EPA acknowledged the importance of using focused studies to develop a PIC list that is (1) appropriately protective of the environment, and (2) not excessively burdensome on the regulated community. Nevertheless, Tables 1 and 2 in U.S. EPA (1994b) were compiled as draft lists for use during the interim period. Tables in U.S. EPA (1994b) were to be revised as additional PIC data were collected. U.S. EPA Permits and State Program Division is currently updating these tables; however, a target completion date is not available. Tables 1 and 2 are based on the following (U.S. EPA 1994b):

- Hazardous waste constituent list in 40 CFR Part 261, Appendix VIII
- hazardous air pollutants (HAP) list
- Office of Research and Development list of organic compounds found in combustion devices developed for U.S. EPA (1993)

The following compounds were deleted from this list:

- Pesticide compounds not likely to be a PIC
- Federal Drug Administration-regulated drugs
- Carcinogenic sugar substitutes
- Compounds without chemical-specific listings (for example, "coal tar")
- Compounds without U.S. EPA-established sampling and analysis methods
- Metallic compounds (because of difficulty in analyzing the specific compounds; metals are still included in elemental totals)

US EPA ARCHIVE DOCUMENT

- Compounds with low octanol-water partition coefficients and no inhalation toxicity data
- Compounds with low toxicity values
- Naturally-occurring plant toxins

Specific compounds were retained on Tables 1 and 2 on the following basis:

- Pesticides with a molecular structure simple enough to be of concern as a PIC
- Compounds with very high octanol-water partition coefficients

A1.8 COLUMN 8: PICS ACTUALLY DETECTED IN STACK EMISSIONS

Compounds marked by an "X" in the appropriate cells are PICs that have actually been detected in stack emissions. U.S. EPA compiled this list by evaluating the studies highlighted in Section A1.6.

US EPA ARCHIVE DOCUMENT

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US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

APPENDIX A-2

COMPOUND SPECIFIC PARAMETER VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX A-2

TABLE OF CONTENTS

Section **Page**

LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS A-2-ii

A2.1 GUIDANCE DOCUMENTS AS PRIMARY REFERENCE SOURCES A-2-1

A2.2 GENERAL ANALYSIS AND METHODOLOGY A-2-2

A2.3 PHYSICAL AND CHEMICAL PROPERTIES A-2-3

A2.3.1 Molecular Weight (*MW*) A-2-3
A2.3.2 Melting Point Temperature (T_m) A-2-4
A2.3.3 Vapor Pressure (*Vp*) and Aqueous Solubility (*S*) A-2-4
A2.3.4 Henry's Law Constant (*H*) A-2-6
A2.3.5 Diffusivity of COPCs in Air (D_a) and Water (D_w) A-2-7
A2.3.6 Octanol-Water Partitioning Coefficient (K_{ow}) A-2-8
A2.3.7 Organic Carbon Partition Coefficient (K_{oc}) A-2-10

A2.3.7.1 Ionizing Organic Compounds A-2-10
A2.3.7.2 Nonionizing Organic Compounds A-2-10

A2.3.8 Partitioning Coefficients for Soil-Water (Kd_s), Suspended Sediment-Surface Water (Kd_{sw}), and Bottom Sediment-Sediment Pore Water (Kd_{bs}) A-2-12
A2.3.9 COPC Soil Loss Constant Due to Biotic and Abiotic Degradation A-2-14
A2.3.10 Fraction of COPC Air Concentration in the Vapor Phase (F_v) A-2-15

REFERENCES A-2-17

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES A-2-25

US EPA ARCHIVE DOCUMENT

APPENDIX A-2

LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

ρ_{air}	=	Density of air (g/cm^3)
ρ_{forage}	=	Density of forage (g/cm^3)
Ba_{beef}	=	Biotransfer factor in beef (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
$Ba_{chicken}$	=	Biotransfer factor in chicken (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{egg}	=	Biotransfer factor in eggs (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{milk}	=	Biotransfer factor in milk (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{pork}	=	Biotransfer factor in pork (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
BAF_{fish}	=	Bioaccumulation factor in fish (mg COPC/kg FW tissue)/(mg COPC/L total water column) OR (L water/kg FW tissue)
BCF_{fish}	=	Bioconcentration factor in fish (L/kg FW OR unitless)
Br_{ag}	=	Plant-soil bioconcentration factor in aboveground produce (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
$Br_{forage/silage}$	=	Plant-soil bioconcentration factor in forage and silage (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
Br_{grain}	=	Plant-soil bioconcentration factor in grain (µg COPC/g DW grain)/(µg COPC/g DW soil)—unitless
$Br_{rootveg}$	=	Plant-soil bioconcentration factor for belowground produce (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
$BSAF_{fish}$	=	Biota-sediment accumulation factor in fish (mg COPC/kg lipid tissue)/(mg COPC/kg sediment)—unitless
B_{vol}	=	Volumetric air-to-leaf biotransfer factor in leaf (µg COPC/L FW plant)/(µg COPC/L air)—unitless
Bv_{ag}	=	COPC air-to-plant biotransfer factor for aboveground produce (µg COPC/g DW plant)/(µg COPC/g air)—unitless
$Bv_{forage/silage}$	=	Air-to-plant biotransfer factor in forage and silage (µg COPC/g DW plant)/(µg COPC/g air)—unitless
c	=	Junge constant = 1.7×10^{-04} (atm-cm)
D_a	=	Diffusivity of COPC in air (cm^2/s)
D_w	=	Diffusivity of COPC in water (cm^2/s)
$f_{oc,bs}$	=	Fraction of organic carbon in bottom sediment (unitless)
$f_{oc,s}$	=	Fraction of organic carbon in soil (unitless)
$f_{oc,sw}$	=	Fraction of organic carbon in suspended sediment (unitless)
f_{water}	=	Fraction of COPC in water (unitless)

US EPA ARCHIVE DOCUMENT

F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Fw	=	Fraction of wet deposition that adheres to plant surfaces (unitless)
H	=	Henry's law constant
Inhalation CSF	=	Inhalation cancer slope factor $(mg/kg\text{-}day)^{-1}$
Inhalation URF	=	Inhalation unit risk factor $(\mu g/m^3)^{-1}$
Kd_s	=	Soil-water partition coefficient (mL water/g soil OR cm^3 water/g soil)
Kd_{sw}	=	Suspended sediment-surface water partition coefficient (L water/kg suspended sediment OR cm^3 water/g suspended sediment)
Kd_{bs}	=	Bed sediment-sediment pore water partition coefficient (L water/kg bottom sediment OR cm^3 water/g bottom sediment)
K_{ow}	=	Octanol/water partitioning coefficient (mg COPC/L octanol)/(mg COPC/L octanol)—unitless
K_{oc}	=	Soil organic carbon-water partition coefficient (mL water/g soil)
ksg	=	COPC soil loss constant due to biotic and abiotic degradation (yr^{-1})
MW	=	Molecular weight of COPC (g/mole)
p°_L	=	Liquidphase vapor pressure of COPC (atm)
p°_S	=	Solid-phase vapor pressure of COPC (atm)
Oral CSF	=	Oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
R	=	Universal gas constant $(atm\text{-}m^3/mol\text{-}K)$
RCF	=	Root concentration factor (µg COPC/g DW plant)/(µg COPC/mL soil water)
RfC	=	Reference concentration (mg/m^3)
RfD	=	Reference dose (mg/kg/day)
Rp	=	Interception factor of edible portion of plant (unitless)
S	=	Solubility of COPC in water (mg COPC/L water)
ΔS_f	=	Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T	=	Whitby's average surface area of particulates (aerosols) = 3.5×10^{-06} cm^2/cm^3 air for background plus local sources = 1.1×10^{-05} cm^2/cm^3 air for urban sources
$t_{1/2}$	=	Half-time of COPC in soil (days)
T_a	=	Ambient air temperature (K)
T_m	=	Melting point temperature (K)
TEF	=	Toxicity equivalency factor (unitless)
Vp	=	Vapor pressure of COPC (atm)

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APPENDIX A-2

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

A2.1 PRIMARY GUIDANCE DOCUMENTS

Throughout Appendix A-2, the following guidance documents are referenced as the primary sources for the development and comparision of compound-specific parameter values, and used to the fullest extent possible to provide consistency. Therefore, in this appendix, the term **primary guidance documents** refers to the following documents:

- U.S. EPA. 1994f. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes: Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response (OERR). Office of Solid Waste. December 14.

- U.S. EPA. 1995b. *Review Draft Development of Human Health Based and Ecologically Based Exit Criteria for the Hazardous Waste Identification Project*. Volumes I and II. Office of Solid Waste. March 3.

- North Carolina Department of Environment, Health, and Natural Resources (NC DEHNR). 1997. *North Carolina Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

To ensure consistency, sources referenced in the primary guidance documents were also evaluated. Information for certain compounds like PCDDs, PCDFs, and mercury were obtained from the following documents:

- U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds*. External Review Draft Report. Volumes I-III. Office of Research and Development. Washington, DC. EPA/600/6-88/005Ca,b,c.

- U.S. EPA. 1997g. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* Office of Air Quality Planning and Standards and Office of Research and Development. EPA-452/R-97-005. December.

U.S. EPA (1994a) provides various parameter values for (but are not limited to) PCDDs, PCDFs, and PCBs. U.S. EPA (1997g) provides various parameter values for mercuric compounds including elemental mercury, mercuric chloride, and methyl mercury.

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A2.2 GENERAL ANALYSIS AND METHODOLOGY

This section describes the general analysis and methodology followed for the development of compound-specific parameter values presented. Compound-specific parameter values in the primary guidance documents and other sources generally were evaluated as follows:

1. Compound-specific values for each parameter were compared among the primary guidance documents and the following observations were noted:

   a. Parameter values provided in U.S. EPA (1994f) are limited to 24 compounds. For these compounds, sources were referenced specifically to each parameter, in addition to the methodology used to obtain the respective values.

   b. U.S. EPA (1995b) provides various parameter values for a comprehensive list of compounds. The methodology used for determining values was covered in detail. However, parameter values for each compound were not referenced to a specific source. Although a comprehensive list of sources was provided, it is difficult to determine which parameter value for a compound was obtained from which source.

   c. NC DEHNR (1997) provides various parameter values for a comprehensive list of compounds, including congeners of polychlorinated dibenzo(p)dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs). However, the sections citing the methodology and sources of values in the NC DEHNR (1997) were reproduced directly from U.S. EPA (1994f). Therefore, in NC DEHNR (1997), the compound-specific parameter values that were provided did not correlate with the sections citing the methodology and sources of values. In addition, only a partial list of sources was provided for the values. Therefore, it was not possible to determine the actual source of values with certainty.

2. Sources of values referenced in the primary guidance documents were further researched and evaluated. Observations affecting usability are included in parameter-specific discussions for each compound, as appropriate.

3. Values provided in the primary guidance documents were used only when the sources and applicability of such values could be verified. Additional sources of parameter values were evaluated, used, and referenced when technically justified.

4. Recommended parameter values obtained using correlations or equations were calculated using the recommended values for these variables provided in this SLERAP.

In general, for the selection of parameter values, the following three steps were followed:

1. Whenever measured parameter values were available in published literature studies, they were preferred for use over other types of data. When multiple measured values were available, the geometric mean of the parameter values is recommended for use.

2. In the absence of measured values in published literature that could not be directly evaluated, parameter values compiled or adopted for use by the primary guidance

US EPA ARCHIVE DOCUMENT

documents, U.S. EPA (1994a), and U.S. EPA (1997g) are recommended.

3. If unable to obtain acceptable values from published literature or the primary guidance documents, parameter values were estimated or calculated using correlation equations based on sound scientific judgment.

The following sections, A2.3 through A2.5, provide compound-specific parameter values, which are categorized and discussed as follows: (1) organic compounds, including polychlorinated biphenyls (PCB), and excluding methyl mercury, PCDDs and PCDFs, (2) PCDDs and PCDFs, (3) all metals except mercury, and (4) the mercuric compounds—mercury (elemental; metal), mercuric chloride (divalent inorganic mercury), and methyl mercury (organic mercury).

For each of the parameters, the sources of values referenced in this SLERAP are followed by a discussion and justification of their selection. There is also a brief discussion of the methodology followed by each of the primary guidance documents. This provides a complete evaluation and comparison of the compound-specific parameter values provided in the primary guidance documents that are currently used to conduct risk assessments.

A2.3 PHYSICAL AND CHEMICAL PROPERTIES

A2.3.1 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, this SLERAP provides *MW* values that 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).

US EPA ARCHIVE DOCUMENT

A2.3.2 Melting Point Temperature (T_m)

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

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, this SLERAP provides values for T_m that 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.

A2.3.3 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 COPC/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 1994c. *Draft Report Chemical Properties for Soil Screening Levels*. Prepared for the Office of Emergency and Remedial Response. Washington, DC. July 26.

U.S. EPA (1994c) provides measured, calculated, and estimated values for *Vp* and *S* that were obtained from various literature sources. *Vp* values in U.S. EPA (1994c) were generally either measured (at 20°C to 25°C) or calculated values obtained from various literature sources. U.S. EPA (1994c), however, provides values for *Vp* corrected to 25°C. U.S. EPA (1995b) 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. The geometric mean of the temperature corrected *Vp* values, determined from measured and calculated values, is recommended for use in this SLERAP.

In U.S. EPA (1994c), *S* values were either measured (at 20°C to 30°C) or calculated values obtained from various literature sources. The geometric mean *S* value, calculated from measured and calculated values, is recommended for use in this SLERAP. Although *S* values were measured at temperatures ranging

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from 20°C to 30°C, U.S. EPA (1994c) 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 (1994c) 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 (1994c) 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 (1994c) were generally consistent with those provided in U.S. EPA (1994f), U.S. EPA (1995b), and NC DEHNR (1997).

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

1. U.S. EPA (1994f)

2. U.S. EPA (1995b); 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. 1994b. *Superfund Chemical Data Matrix (SCDM).* Office of Emergency and Remedial Response. Washington, DC. June.

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

Most *Vp* and *S* values in U.S. EPA (1995b) 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 (1994b) were obtained from various literature sources. *S* values in U.S. EPA (1994b) were the geometric mean of values obtained from various literature sources.

PCDDs and PCDFs *Vp* and *S* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). *Vp* and *S* values were either (1) measured, or (2) estimated by using the homologue (compound class with the same amount of chlorination) average method.

US EPA ARCHIVE DOCUMENT

NOTE: The phase—solid or liquid—of *Vp* values for all organics, including PCDDs and PCDFs, was indicated. This is based on whether the compound is in the solid or liquid phase at ambient soil temperatures.

Metals As cited in the primary guidance documents and in the literature, metals—except mercury—are considered (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids. Therefore, *Vp* and *S* values were not available for all metals (except mercury) in any of the literature sources reviewed.

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); and are comparable to the values in the primary guidance documents. *Vp* and *S* values for mercuric chloride were obtained from U.S. EPA (1997g) and Budavari, O'Neil, Smith, and Heckelman (1989), respectively. *Vp* and *S* values for methyl mercury were not found in the literature.

A2.3.4 Henry's Law Constant (*H*)

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentation of the compound in water at a given temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure. Experimental and estimated *H* values from literature reports, however, are (1) very temperature-dependent and difficult to measure, (2) generally obtained from various literature sources that use different experimental and estimation methods, and (3) available for only a limited number of compounds.

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

$$H = \frac{Vp \cdot MW}{S} \qquad \text{Equation A2-1}$$

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

The primary guidance documents also used theoretical Equation A-3-1 to calculate *H* values.

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

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

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

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A2.3.5 Diffusivity of COPCs 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 COPC into a waterbody.

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

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

The U.S. EPA (1994d) database uses empirical correlations with compound density and molecular weight to calculate diffusivity values. For compounds not in the U.S. EPA (1994d) 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(1995d) database values were predicted by using chemical-structural relationships. Diffusivity values for all compounds in the U.S. EPA (1994d) and (1995d) databases were either predicted or estimated. The primary guidance documents also recommended U.S. EPA (1994d) and (1995d) database model values. More recent documents, including the following, also recommended these values:

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

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

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}} \qquad \text{Equation A2-2a}$$

$$D_{w,i} = \frac{22\times10^{-5}}{(MW_i)^{2/3}} \qquad \text{Equation A2-2b}$$

U.S. EPA (1995b) recommended the use of standard default diffusivity values. U.S. EPA (1995b) 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 (1995b) 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 (1995b) recommended a default value of 8 x 10^{-06} cm^2/s. Diffusivity values calculated using Equations A-2-2a and A-2-2b were within the range specified by U.S. EPA (1995b), and therefore, were adopted for use in this SLERAP.

US EPA ARCHIVE DOCUMENT

PCDDs and PCDFs Diffusivity values in air and water for (1) 2,3,7,8-TCDD were obtained from U.S. EPA (1994e), and (2) 2,3,7,8-TCDF were obtained from U.S. EPA (1995d). For all other congeners of PCDDs and PCDFs, (1) a default *Dw* value of 8×10^{-06} cm^2/s was used, and (2) *Da* values were calculated using the following equation recommended by U.S. EPA (1994a):

$$\frac{D_x}{D_y} = \left(\frac{MW_y}{MW_x}\right)^{0.5} \qquad \text{Equation A2-2c}$$

where

$D_{x,y}$ = Diffusivities in air of compounds *x* and *y* (cm^2/s)
$MW_{x,y}$ = Molecular weights of compounds *x* and *y* (g/mol)

Da values for PCDD congeners were calculated by using the *Da* value and *MW* for 2,3,7,8-TCDD. *Da* values for PCDF congeners were calculated using the *Da* value and *MW* for 2,3,7,8-TCDF. This approach is consistent with the methodology specified in U.S. EPA (1994a).

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 (1994d) database. Diffusivity values for mercuric chloride and methyl mercury were calculated using Equations A-2-2a and A-2-2b.

A2.3.6 Octanol/Water Partitioning Coefficient (K_{ow})

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

Organics For organics (except PCDDs and PCDFs), K_{ow} values were obtained from U.S. EPA (1994c). U.S. EPA (1994c) provides measured, calculated, and estimated K_{ow} values obtained from various literature sources. The geometric mean K_{ow} value, calculated from all measured and calculated values for each compound, is recommended in this SLERAP.

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

1. U.S. EPA (1994f)

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

US EPA ARCHIVE DOCUMENT

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

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

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

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

U.S. EPA (1994c) is the preferred source of values because (1) sources were provided, (2) several literature values were provided, some of which are also cited by the primary guidance documents and Karickhoff and Long (1995), and (3) the values were provided to 2 significant figures.

U.S. EPA (1994f) is the second-choice source of K_{ow} values recommended; and provides geometric mean values obtained from various literature sources. Karickhoff and Long (1995) recommended arithmetic mean values obtained from various literature sources and was, therefore, preferred as the third-choice source of K_{ow} values when values were not available from the first two sources.

In order to reference specific sources of K_{ow} values for each compound, values from U.S. EPA (1995b) and NC DEHNR (1997) were used only when values were not available in the literature sources reviewed.

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

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

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

US EPA ARCHIVE DOCUMENT

A2.3.7 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.

A2.3.7.1 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 (1994c). U.S. EPA (1994c) 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. Therefore, for the aforementioned ionizing organic compounds, this SLERAP prefers and provides estimated K_{oc} values that are based on pH.

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 (1994c), for low pH conditions, these estimated values may overpredict sorption coefficients, because they ignore sorption to components other than organic carbon.

A2.3.7.2 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. This SLERAP uses geometric mean of measured K_{oc} values provided in the following document:

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

US EPA ARCHIVE DOCUMENT

NC DEHNR (1997) and U.S. EPA (1994f) use the following correlation equation to calculate K_{oc} from K_{ow} for all organics:

$$\log K_{oc} = 0.88 (\log K_{ow}) + 0.114 \qquad (r^2 = 0.96) \qquad \text{Equation A-2-3}$$

- Research Triangle Institute (RTI). 1992. *Preliminary Soil Action Level for Superfund Sites, Draft Interim Report.* Prepared for U.S. EPA Hazardous Site Control Division, Remedial Operations Guidance Branch. Arlington, Virginia. December.

However, according to U.S. EPA (1994c), the correlation between K_{oc} and K_{ow} can be improved considerably by performing separate linear regressions on two chemical groups. U.S. EPA (1994c) derives the following correlation equations from measured K_{oc} values cited in U.S. EPA (1994c) and U.S. EPA (1996b):

For phthalates and PAHs

$$\log K_{oc} = 0.97 (\log K_{ow}) - 0.094 \qquad (r^2 = 0.99) \qquad \text{Equation A-2-4}$$

For all organics except phthalates, PAHs, PCDDs, and PCDFs

$$\log K_{oc} = 0.78 (\log K_{ow}) + 0.151 \qquad (r^2 = 0.98) \qquad \text{Equation A-2-5}$$

Because of the improved regressions (r^2), U.S. EPA (1994c) recommended that correlation Equations A-2-4 and A-2-5 be used instead of correlation Equation A-2-3. U.S. EPA (1995b) also recommended that correlation Equations A-2-4 and A-2-5 be used.

Although U.S. EPA (1995b) recommended the use of correlation Equations A-2-4 and A-2-5, the following correlation equation was used by that document to calculate K_{oc} values for all organics except PCDDs and PCDFs:

$$\log K_{oc} = 0.983 (\log K_{ow}) + 0.0002 \qquad \text{Equation A-2-6}$$

- DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas, and P.R. Paquin. 1991. "Technical Basis for

US EPA ARCHIVE DOCUMENT

Establishing Sediment Quality Criteria for Nonionic Compounds Using Equilibrium Partitioning." *Environmental Toxicology and Chemistry*. 10:1541-1583

For the purposes of this SLERAP, values obtained by using correlation Equations A-2-3 through A-2-6, were compared. In general, more of the K_{oc} values obtained by using correlation Equations A-2-4 and A-2-5 were within the range of measured values in the literature than those obtained by using correlation Equations A-2-3 and A-2-6. Therefore, when measured K_{oc} values were not available, values were estimated, for all nonionizing organic compounds except PCDDs and PCDFs, by using the appropriate correlation Equation A-2-4 or A-*2-5*.

PCDDs and PCDFs For PCDDs and PCDFs, the following correlation equation (Karickhoff, Brown, and Scott 1979) was used to calculate K_{oc} values, as cited by U.S. EPA (1994a).

$$\log K_{oc} = \log K_{ow} - 0.21 \qquad (n = 10,\ r^2 = 1.0) \qquad \text{Equation A-2-7}$$

- Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. "Sorption of Hydrophobic Pollutants on Natural Sediments." Water Resources. 13:241-248.

Metals For metals, no K_{oc} values were found in the literature. K_{oc} values for metals were not provided in the primary guidance documents, because of the stated assumption that organic carbon in soils does not play a major role in partitioning in soil and sediments. For metals, soil/sediment-water partitioning coefficients (*Kd*) were obtained directly from experimental measurements (see *Kd* discussion).

Note: For compounds in which a K_{ow} correlation equation was used to calculate a K_{oc} value, K_{ow} values recommended for each compound in this SLERAP were used.

A2.3.8 Partitioning Coefficients for Soil-Water (Kd_s), Suspended Sediment-Surface Water (Kd_{sw}), and Bottom Sediment-Sediment Pore Water (Kd_{bs})

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. The bed sediment-sediment pore-water partition coefficient (Kd_{bs}) coefficient describes the partitioning of a compound between the bed sediments and bed sediment pore-water.

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:

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$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-2-8a}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-2-8b}$$

$$Kd_{bs} = f_{oc,bs} \cdot K_{oc} \qquad \text{Equation A-2-8c}$$

- U.S. EPA. 1993d. 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.
- 0.03 to 0.05 in bottom sediments—for which a mid-range value of $f_{oc,bs}$ = 0.04 generally can be used.

Consistent with the primary guidance documents, this SLERAP uses mid-range f_{oc} values recommended by U.S. EPA (1993d). *Kd* values were calculated using K_{oc} values recommended for each compound in this SLERAP.

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 (1996b). U.S. EPA (1996b) 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.

U.S. EPA (1995b) also recommended *Kd* values estimated using the MINTEQ2 model. U.S. EPA (1994f) and NC DEHNR (1997) provided *Kd* values obtained from several literature sources, depending on the compound; however, the *Kd* values are identical in all of the primary guidance documents.

The MINTEQ2 model values in U.S. EPA (1996b) were comparable to the values in the primary guidance documents. In addition, because organic carbon does not play a major role in partitioning for the metals, U.S. EPA (1994f) assumed that the partitioning is the same, regardless of the soil, suspended

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sediment, or bottom sediment phase. Therefore, in this SLERAP, values for partitioning coefficients Kd_s, Kd_{sw}, and Kd_{bs} for the metals are assumed to be the same.

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 Kd_s, Kd_{sw}, and Kd_{bs} values for mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1996b). Kd values for mercuric chloride and methyl mercury were obtained from U.S. EPA (1997g).

A2.3.9 Soil Loss Constant Due to Degradation *(ksg)*

Soil loss constant due to degradation *(ksg)* reflects loss of a compound from the soil by processes other than leaching. Degradation rates in the soil media include biotic and abiotic mechanisms of transformation. Abiotic degradation includes photolysis, hydrolysis, and redox reactions. Hydrolysis and redox reactions can be significant abiotic mechanisms in soil (U.S. EPA 1990).

The following document states that degradation rates can be assumed to follow first order kinetics in a homogenous media:

- Lyman , W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds.* McGraw-Hill Book Company. New York, New York.

Therefore, the half-life $(t_{½})$ of compounds can be related to the degradation rate constant (*ksg*) as follows:

$$ksg = \frac{0.693}{t_{½}} \qquad \text{Equation A-2-9}$$

Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil. Therefore, if the $t_{½}$ for all of the mechanisms of transformation are known, the degradation rate can be calculated using Equation A-2-9. However, literature sources generally do not provide sufficient data for all such mechanisms, especially for soil.

Organics For organics (except PCDDs and PCDFs), *ksg* values were calculated using half-life soil values obtained from the following document:

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

Half-life values provided in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) indicate the disappearance of a substance in ground water or soil; with the principal degradation mechanisms being

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biodegradation and hydrolysis. Values reported were highly variable because of the different methods used for measurements, in addition to the various controlling factors that could affect them. Therefore, Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) provided a range of half-life values found in the literature, usually for the fastest reaction mechanism,. *Ksg* values recommended in this SLERAP were calculated with the high-end half-life values.

U.S. EPA (1994b) also cited values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991). NC DEHNR (1997) cited values that are comparable to *ksg* values calculated by using half-life values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).

PCDDs and PCDFs For PCDDs and PCDFs, *ksg* values were calculated from half-life values in soil obtained from Mackay, Shiu, and Ma (1992). For 2,3,7,8-TCDD, *ksg* value was obtained from U.S. EPA (1994a); which discussed experimental studies that were conducted on PCDDs and PCDFs degradation mechanisms. U.S. EPA (1994a) summarized the degradation of PCDDs and PCDDs as follows:

- A few experimental studies have shown possible biological degradation of TCDDs. However, the studies conclude that microbial action is very slow for PCDDs under optimum conditions, with the degradation rates probably higher with decreasing chlorination. PCDFs were found to be extremely stable to biological degradation.

- Abiotic degradation, such as photolysis, appears to be the most significant natural degradation mechanism for PCDDs and PCDFs. Experimental studies have shown that PCDDs and PCDFs undergo photolysis in the presence of a suitable hydrogen donor. No information was available to show that other abiotic degradation mechanisms, such as oxidation and hydrolysis, are important under environmentally relevant conditions.

Metals For the metals, NC DEHNR (1997) cites *ksg* values of zero. Literature states that the metals are transformed, but not degraded, by such mechanisms; therefore, *ksg* values are not applicable to metals.

Mercuric Compounds For mercury, mercuric chloride, and methylmercury, U.S. EPA (1997g) recommended *ksg* values of zero.

A2.3.10 Fraction of Pollutant Air Concentration in the Vapor Phase (F_v)

Organics For organics, the fraction of pollutant air concentration in the vapor phase (F_v) was calculated using the following equation:

$$Fv = 1 - \frac{c\,S_T}{p^{\circ}_L + c\,S_T} \qquad \text{Equation A-2-10}$$

- Junge, C. E. 1977. *Fate of Pollutants in the Air and Water Environments*, Part I; Suffet, I. H., Ed.; Wiley; New York. Pages 7-26.

If the compound is a liquid at ambient temperatures (that is, when p°_L is known), Equation A-2-10 calculates F_v using the vapor pressure value recommended for that compound in this SLERAP. If the

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compound is a solid at ambient temperatures (that is, when p°_S is known), the following equation (Bidleman 1988) was used to calculate p°_L from p°_S, for use in Equation A-2-10:

$$\ln\left(\frac{p^{\circ}_L}{p^{\circ}_S}\right) = \frac{\Delta S_f}{R}\,\frac{(T_m - T)}{T} \qquad \text{Equation A-2-11}$$

where

c	=	Junge constant = 1.7 x 10^{-04} (atm-cm)
p°_L	=	Liquid phase vapor pressure of compound (atm)
p°_s	=	Solid phase vapor pressure of compound (atm)
R	=	Universal ideal gas constant (atm-m^3/mole-K)
ΔS_f	=	Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T	=	Whitby's average surface area of particulates (aerosols)
T_a	=	Ambient air temperature (K)—assumed to be 25°C or 298 K

This equation was adopted from:

- Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Number 4. Pages 361-367.

According to Bidleman (1988), Equation A-2-10 assumes that the Junge constant (*c*) is constant for all compounds. However, *c* can depend on (1) the compound (sorbate) molecular weight, (2) the surface concentration for monolayer coverage, and (3) the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate.

The primary guidance documents used Equations A-2-10 and A-2-11 to compute *Fv*. However, it is not clear what values of *S*, *T*, and *Vp* values were used to calculate values for F_v. For example, U.S. EPA (1994f) calculated F_v values at (*T*) of 11°C. Because of inconsistencies in the values in the primary guidance documents, *Fv* values in the primary guidance documents were not recommended for use in this SLERAP. F_v values were calculated using the recommended values of *Vp* and T_m provided in this SLERAP for each compound.

Metals Consistent with U.S. EPA (1994f), all metals (except mercury) are assumed to be present in the particulate phase and not in the vapor phase (*Vp* = 0), and assigned F_v values of zero.

Mercuric Compounds Mercury and mercuric chloride are relatively volatile and exist in the vapor phase (U.S. EPA 1997g). Therefore, the *Fv* value recommended in this SLERAP for mercury was calculated using Equations A-2-10 and A-2-11.

Based on discussions on mercury presented in Chapter 2 of this SLERAP, *Fv* values of 1.0 for mercury (same as calculated using Equations A-2-10 and A-2-11), and 0.85 for mercuric chloride were estimated. Consistent with information provided in U.S. EPA (1997g), methyl mercury is assumed not to exist in the air phase and, therefore, assigned an *Fv* of zero.

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US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 1 of 10)

Table			Page
A-2-1	CAS NUMBER 83-32-9:	ACENAPHTHENE	A-2-35
A-2-2	CAS NUMBER 75-07-0:	ACETALDEHYDE	A-2-36
A-2-3	CAS NUMBER 67-64-1:	ACETONE	A-2-37
A-2-4	CAS NUMBER 75-05-8:	ACETONITRILE	A-2-38
A-2-5	CAS NUMBER 98-86-2:	ACETOPHENONE	A-2-39
A-2-6	CAS NUMBER 107-02-8:	ACROLEIN	A-2-40
A-2-7	CAS NUMBER 107-13-1:	ACRYLONITRILE	A-2-41
A-2-8	CAS NUMBER 309-00-2:	ALDRIN	A-2-42
A-2-8a	CAS NUMBER 7429-90-5:	ALUMINUM	A-2-43
A-2-9	CAS NUMBER 62-53-3:	ANILINE	A-2-44
A-2-10	CAS NUMBER 120-12-7:	ANTHRACENE	A-2-45
A-2-11	CAS NUMBER 7440-36-0:	ANTIMONY	A-2-46
A-2-12	CAS NUMBER 12674-11-2:	AROCLOR 1016	A-2-47
A-2-13	CAS NUMBER 11097-69-1:	AROCLOR 1254	A-2-48
A-2-14	CAS NUMBER 7440-38-2:	ARSENIC	A-2-49
A-2-15	CAS NUMBER 1912-24-9:	ATRAZINE	A-2-50
A-2-16	CAS NUMBER 7440-36-3:	BARIUM	A-2-51
A-2-17	CAS NUMBER 100-52-7:	BENZALDEHYDE	A-2-52
A-2-18	CAS NUMBER 71-43-2:	BENZENE	A-2-53
A-2-19	CAS NUMBER 56-55-3:	BENZO(A)ANTHRACENE	A-2-54
A-2-20	CAS NUMBER 50-32-8:	BENZO(A)PYRENE	A-2-55

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 2 of 10)

A-2-21	CAS NUMBER 205-99-2:	BENZO(B)FLUORANTHENE	A-2-56
A-2-22	CAS NUMBER 207-08-9:	BENZO(K)FLUORANTHENE	A-2-57
A-2-23	CAS NUMBER 65-85-0:	BENZOIC ACID	A-2-58
A-2-24	CAS NUMBER 100-47-0:	BENZONITRILE	A-2-60
A-2-25	CAS NUMBER 100-51-6:	BENZYL ALCOHOL	A-2-61
A-2-26	CAS NUMBER 100-44-7:	BENZYL CHLORIDE	A-2-62
A-2-27	CAS NUMBER 7440-41-7:	BERYLLIUM	A-2-63
A-2-28	CAS NUMBER 319-84-6:	BHC, ALPHA-	A-2-64
A-2-29	CAS NUMBER 319-85-7:	BHC, BETA-	A-2-65
A-2-30	CAS NUMBER 111-44-4:	BIS(2-CHLORETHYL)ETHER	A-2-66
A-2-31	CAS NUMBER 75-27-4:	BROMODICHLOROMETHANE	A-2-67
A-2-32	CAS NUMBER 75-25-2:	BROMOFORM (TRIBROMOMETHANE)	A-2-68
A-2-33	CAS NUMBER 101-55-3:	BROMOPHENYL-PHENYLETHER, 4-	A-2-69
A-2-34	CAS NUMBER 85-68-7:	BUTYLBENZYLPHTHALATE	A-2-70
A-2-35	CAS NUMBER 7440-43-9:	CADMIUM	A-2-71
A-2-36	CAS NUMBER 75-15-0:	CARBON DISULFIDE	A-2-72
A-2-37	CAS NUMBER 56-23-5:	CARBON TETRACHLORIDE	A-2-73
A-2-38	CAS NUMBER 57-74-9:	CHLORDANE	A-2-74
A-2-39	CAS NUMBER 7782-50-5:	CHLORINE	A-2-75
A-2-40	CAS NUMBER 59-50-7:	CHLORO-3-METHYLPHENOL, 4-	A-2-76
A-2-41	CAS NUMBER 106-47-8:	CHLOROANILINE, p-	A-2-77

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 3 of 10)

A-2-42	CAS NUMBER 108-90-7:	CHLOROBENZENE	A-2-78
A-2-43	CAS NUMBER 510-15-6:	CHLOROBENZILATE	A-2-79
A-2-44	CAS NUMBER 75-45-6:	CHLORODIFLUOROMETHANE	A-2-80
A-2-45	CAS NUMBER 75-00-3:	CHLOROETHANE	A-2-81
A-2-46	CAS NUMBER 67-66-3:	CHLOROFORM (TRICHLOROMETHANE)	A-2-82
A-2-47	CAS NUMBER 39638-32-9:	CHLOROISOPROPYL ETHER, BIS-1,2-	A-2-83
A-2-48	CAS NUMBER 91-58-7:	CHLORONAPHTHALENE, 2-	A-2-84
A-2-49	CAS NUMBER 95-57-8:	CHLOROPHENOL, 2-	A-2-85
A-2-50	CAS NUMBER 7005-72-3:	CHLOROPHENYL-PHENYLETHER, 3-	A-2-87
A-2-51	CAS NUMBER 2921-88-2:	CHLOROPYRIFOS	A-2-88
A-2-52	CAS NUMBER 7440-47-3:	CHROMIUM	A-2-89
A-2-53	CAS NUMBER 18540-29-9:	CHROMIUM, HEXAVALENT	A-2-90
A-2-54	CAS NUMBER 218-01-9:	CHRYSENE	A-2-91
A-2-54a	CAS NUMBER 7440-50-8:	COPPER	A-2-92
A-2-55	CAS NUMBER 108-39-4:	CRESOL, m-	A-2-93
A-2-56	CAS NUMBER 95-48-7:	CRESOL, o-	A-2-94
A-2-57	CAS NUMBER 106-44-5:	CRESOL, p-	A-2-95
A-2-58	CAS NUMBER 98-82-8:	CUMENE (ISOPROPYLBENZENE)	A-2-96
A-2-59	CAS NUMBER 57-12-5:	CYANIDE	A-2-97
A-2-60	CAS NUMBER 72-54-8:	DDD, 4,4'-	A-2-98
A-2-61	CAS NUMBER 72-55-9:	DDE, 4,4'-	A-2-99

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 4 of 10)

A-2-62	CAS NUMBER 50-29-3:	DDT, 4,4'-	A-2-100
A-2-63	CAS NUMBER 84-74-2:	DI-N-BUTYL PHTHALATE	A-2-101
A-2-64	CAS NUMBER 117-84-0:	DI(N-OCTYL) PHTHALATE	A-2-102
A-2-65	CAS NUMBER 333-41-5:	DIAZINON	A-2-103
A-2-66	CAS NUMBER 53-70-3:	DIBENZO(A,H)ANTHRACENE	A-2-104
A-2-67	CAS NUMBER 96-12-8:	DIBROMO-3-CHLOROPROPANE 1,2-	A-2-105
A-2-68	CAS NUMBER 124-48-1:	DIBROMOCHLOROMETHANE	A-2-106
A-2-69	CAS NUMBER 95-50-1:	DICHLOROBENZENE, 1,2-	A-2-107
A-2-70	CAS NUMBER 541-73-1:	DICHLOROBENZENE, 1,3-	A-2-108
A-2-71	CAS NUMBER 106-46-7:	DICHLOROBENZENE, 1,4-	A-2-109
A-2-72	CAS NUMBER 91-94-1:	DICHLOROBENZIDINE, 3,3'-	A-2-110
A-2-73	CAS NUMBER 75-71-8:	DICHLORODIFLUOROMETHANE	A-2-111
A-2-74	CAS NUMBER 75-34-3:	DICHLOROETHANE, 1,1-	A-2-112
A-2-75	CAS NUMBER 107-06-2:	DICHLOROETHANE, 1,2- (ETHYLENE DICHLORIDE)	A-2-113
A-2-76	CAS NUMBER 75-35-4:	DICHLOROETHYLENE, 1,1-	A-2-114
A-2-77	CAS NUMBER 156-59-2:	DICHLOROETHYLENE, CIS-1,2-	A-2-115
A-2-78	CAS NUMBER 156-60-5:	DICHLOROETHYLENE, 1,2(TRANS)-	A-2-116
A-2-79	CAS NUMBER 120-83-2:	DICHLOROPHENOL, 2,4-	A-2-117
A-2-80	CAS NUMBER 78-87-5:	DICHLOROPROPANE, 1,2-	A-2-119
A-2-81	CAS NUMBER 542-75-6:	DICHLOROPROPENE, 1,3(CIS)-	A-2-120
A-2-82	CAS NUMBER 62-73-7:	DICHLORVOS	A-2-121

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 5 of 10)

A-2-83	CAS NUMBER 60-57-1:	DIELDRIN	A-2-122
A-2-84	CAS NUMBER 84-66-2:	DIETHYL PHTHALATE	A-2-123
A-2-85	CAS NUMBER 131-11-3:	DIMETHYL PHTHALATE	A-2-124
A-2-86	CAS NUMBER 105-67-9:	DIMETHYLPHENOL, 2,4-	A-2-125
A-2-87	CAS NUMBER 119-90-4:	DIMETHYOXYBENZIDINE, 3,3'	A-2-127
A-2-88	CAS NUMBER 99-65-0:	DINITROBENZENE, 1,3-	A-2-128
A-2-89	CAS NUMBER 51-28-5:	DINITROPHENOL, 2,4-	A-2-129
A-2-90	CAS NUMBER 121-14-2:	DINITROTOLUENE, 2,4-	A-2-131
A-2-91	CAS NUMBER 606-20-2:	DINITROTOLUENE, 2,6-	A-2-132
A-2-92	CAS NUMBER 123-91-1:	DIOXANE, 1,4-	A-2-133
A-2-93	CAS NUMBER 122-66-7:	DIPHENYLHYDRAZINE, 1,2-	A-2-134
A-2-94	CAS NUMBER 298-04-4:	DISULFOTON	A-2-135
A-2-95	CAS NUMBER 115-29-7:	ENDOSULFAN I	A-2-136
A-2-96	CAS NUMBER 72-20-8:	ENDRIN	A-2-137
A-2-97	CAS NUMBER 106-89-8:	EPICHLOROHYDRIN (1-CHLORO-2,3-EPOXYPROPANE)	A-2-138
A-2-98	CAS NUMBER 97-68-2:	ETHYL METHACRYLATE	A-2-139
A-2-99	CAS NUMBER 62-50-0:	ETHYL METHANESULFONATE	A-2-140
A-2-100	CAS NUMBER 100-41-4:	ETHYLBENZENE	A-2-141
A-2-101	CAS NUMBER 106-93-4:	ETHYLENE DIBROMIDE	A-2-142
A-2-102	CAS NUMBER 75-21-8:	ETHYLENE OXIDE	A-2-143
A-2-103	CAS NUMBER 117-81-7:	ETHYLHEXYL PHTHALATE, BIS-2-	A-2-144

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 6 of 10)

A-2-104	CAS NUMBER 206-44-0:	FLUORANTHENE	A-2-145
A-2-105	CAS NUMBER 86-73-7:	FLUORENE	A-2-146
A-2-106	CAS NUMBER 50-00-0:	FORMALDEHYDE	A-2-147
A-2-107	CAS NUMBER 64-18-6:	FORMIC ACID	A-2-148
A-2-108	CAS NUMBER 35822-46-9:	HEPTACDD, 1,2,3,4,6,7,8-	A-2-149
A-2-109	CAS NUMBER 67562-39-4:	HEPTACDF, 1,2,3,4,6,7,8-	A-2-150
A-2-110	CAS NUMBER 55673-89-7:	HEPTACDF, 1,2,3,4,7,8,9-	A-2-151
A-2-111	CAS NUMBER 76-44-8:	HEPTACHLOR	A-2-152
A-2-112	CAS NUMBER 1024-57-3:	HEPTACHLOR EPOXIDE	A-2-153
A-2-113	CAS NUMBER 39227-28-6:	HEXACDD, 1,2,3,4,7,8-	A-2-154
A-2-114	CAS NUMBER 57653-85-7:	HEXACDD, 1,2,3,6,7,8-	A-2-155
A-2-115	CAS NUMBER 19408-74-3:	HEXACDD, 1,2,3,7,8,9-	A-2-156
A-2-116	CAS NUMBER 70648-26-9:	HEXACDF, 1,2,3,4,7,8-	A-2-157
A-2-117	CAS NUMBER 57117-44-9:	HEXACDF, 1,2,3,6,7,8-	A-2-158
A-2-118	CAS NUMBER 72918-21-9:	HEXACDF, 1,2,3,7,8,9-	A-2-159
A-2-119	CAS NUMBER 60851-34-5:	HEXACDF, 2,3,4,6,7,8-	A-2-160
A-2-120	CAS NUMBER 87-68-3:	HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE)	A-2-161
A-2-121	CAS NUMBER 118-74-1:	HEXACHLOROBENZENE	A-2-162
A-2-122	CAS NUMBER 77-47-4:	HEXACHLOROCYCLOPENTADIENE	A-2-163
A-2-123	CAS NUMBER 67-72-1:	HEXACHLOROETHANE (PERCHLOROETHANE)	A-2-164
A-2-124	CAS NUMBER 70-30-4:	HEXACHLOROPHENE	A-2-165

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 7 of 10)

A-2-125	CAS NUMBER 7647-01-0:	HYDROGEN CHLORIDE	A-2-166
A-2-126	CAS NUMBER 193-39-5:	INDENO(1,2,3-CD)PYRENE	A-2-167
A-2-127	CAS NUMBER 78-59-1:	ISOPHORONE	A-2-168
A-2-128	CAS NUMBER 7439-92-1:	LEAD	A-2-169
A-2-129	CAS NUMBER 121-75-5:	MALATHIONE	A-2-170
A-2-130	CAS NUMBER 7487-94-7:	MERCURIC CHLORIDE	A-2-171
A-2-131	CAS NUMBER 7439-97-6:	MERCURY	A-2-172
A-2-132	CAS NUMBER 126-98-7:	METHACRYLONITRILE	A-2-173
A-2-133	CAS NUMBER 67-56-1:	METHANOL	A-2-174
A-2-134	CAS NUMBER 72-43-5:	METHOXYCHLOR	A-2-175
A-2-135	CAS NUMBER 79-20-9:	METHYL ACETATE	A-2-176
A-2-136	CAS NUMBER 74-83-9:	METHYL BROMIDE (BROMOMETHANE)	A-2-177
A-2-137	CAS NUMBER 74-87-3:	METHYL CHLORIDE (CHLOROMETHANE)	A-2-178
A-2-138	CAS NUMBER 78-93-3:	METHYL ETHYL KETONE (2-BUTANONE)	A-2-179
A-2-139	CAS NUMBER 108-10-1:	METHYL ISOBUTYL KETONE	A-2-180
A-2-140	CAS NUMBER 22967-92-6:	METHYL MERCURY	A-2-181
A-2-141	CAS NUMBER 298-00-0:	METHYL PARATHION	A-2-182
A-2-142	CAS NUMBER 74-95-3:	METHYLENE BROMIDE	A-2-183
A-2-143	CAS NUMBER 75-09-2:	METHYLENE CHLORIDE	A-2-184
A-2-144	CAS NUMBER 91-20-3:	NAPHTHALENE	A-2-185

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 8 of 10)

A-2-145	CAS NUMBER 7440-02-0:	NICKEL	A-2-186
A-2-146	CAS NUMBER 88-74-4:	NITROANILINE, 2-	A-2-187
A-2-147	CAS NUMBER 99-09-2:	NITROANILINE, 3-	A-2-188
A-2-148	CAS NUMBER 100-01-6:	NITROANILINE, 4-	A-2-189
A-2-149	CAS NUMBER 98-95-3:	NITROBENZENE	A-2-190
A-2-150	CAS NUMBER 88-75-5:	NITROPHENOL, 2-	A-2-191
A-2-151	CAS NUMBER 100-02-7:	NITROPHENOL, 4-	A-2-192
A-2-152	CAS NUMBER 924-16-3:	NITROSO-DI-N-BUTYLAMINE, N-	A-2-193
A-2-153	CAS NUMBER 86-30-6:	NITROSODIPHENYLAMINE, N-	A-2-194
A-2-154	CAS NUMBER 621-64-7:	NITROSODIPROPYLAMINE, N	A-2-195
A-2-155	CAS NUMBER 3268-87-9:	OCTACDD, 1,2,3,4,6,7,8,9-	A-2-196
A-2-156	CAS NUMBER 39001-02-0:	OCTACDF, 1,2,3,4,6,7,8,9-	A-2-197
A-2-157	CAS NUMBER 40321-76-4:	PENTACDD, 1,2,3,7,8-	A-2-198
A-2-158	CAS NUMBER 57117-41-6:	PENTACDF, 1,2,3,7,8-	A-2-199
A-2-159	CAS NUMBER 57117-31-4:	PENTACDF, 2,3,4,7,8-	A-2-200
A-2-160	CAS NUMBER 608-93-5:	PENTACHLOROBENZENE	A-2-201
A-2-161	CAS NUMBER 82-68-8:	PENTACHLORONITROBENZENE (PCNB)	A-2-202
A-2-162	CAS NUMBER 87-86-5:	PENTACHLOROPHENOL	A-2-203
A-2-163	CAS NUMBER 85-01-8:	PHENANTHRENE	A-2-205
A-2-164	CAS NUMBER 108-95-2:	PHENOL	A-2-206

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 9 of 10)

A-2-165	CAS NUMBER 298-02-2:	PHORATE	A-2-208
A-2-166	CAS NUMBER 85-44-9:	PHTHALIC ANHYDRIDE (1,2-BENZENE DICARBOXYLIC ANHYDRIDE)	A-2-209
A-2-167	CAS NUMBER 23950-58-5:	PRONAMIDE	A-2-210
A-2-168	CAS NUMBER 129-00-0:	PYRENE	A-2-211
A-2-169	CAS NUMBER 110-86-1:	PYRIDINE	A-2-212
A-2-170	CAS NUMBER 299-84-3:	RONNEL	A-2-213
A-2-171	CAS NUMBER 94-59-1:	SAFROLE	A-2-214
A-2-172	CAS NUMBER 7782-49-2:	SELENIUM	A-2-215
A-2-173	CAS NUMBER 7440-22-4:	SILVER	A-2-216
A-2-174	CAS NUMBER 57-24-9:	STRYCHNINE	A-2-217
A-2-175	CAS NUMBER 100-42-5:	STYRENE	A-2-218
A-2-176	CAS NUMBER 1746-01-6:	TETRACDD, 2,3,7,8-	A-2-219
A-2-177	CAS NUMBER 51207-31-9:	TETRACDF, 2,3,7,8-	A-2-220
A-2-178	CAS NUMBER 95-94-3:	TETRACHLOROBENZENE, 1,2,4,5-	A-2-221
A-2-179	CAS NUMBER 630-20-6:	TETRACHLOROETHANE, 1,1,1,2-	A-2-222
A-2-180	CAS NUMBER 79-34-5:	TETRACHLOROETHANE, 1,1,2,2-	A-2-223
A-2-181	CAS NUMBER 127-18-4:	TETRACHLOROETHYLENE (PERCHLOROETHYLENE)	A-2-224
A-2-182	CAS NUMBER 58-90-2:	TETRACHLOROPHENOL, 2,3,4,6-	A-2-225
A-2-183	CAS NUMBER 109-99-9:	TETRAHYDROFURAN	A-2-227
A-2-184	CAS NUMBER 7440-28-0:	THALLIUM (L)	A-2-228

US EPA ARCHIVE DOCUMENT

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 10 of 10)

A-2-185	CAS NUMBER 108-88-3:	TOLUENE	A-2-229
A-2-186	CAS NUMBER 95-53-4:	TOLUIDINE, o-	A-2-230
A-2-187	CAS NUMBER 87-61-6:	TRICHLOROBENZENE, 1,2,3-	A-2-231
A-2-188	CAS NUMBER 120-82-1:	TRICHLOROBENZENE, 1,2,4-	A-2-232
A-2-189	CAS NUMBER 71-55-6:	TRICHLOROETHANE, 1,1,1-	A-2-233
A-2-190	CAS NUMBER 79-00-5:	TRICHLOROETHANE, 1,1,2-	A-2-234
A-2-191	CAS NUMBER 79-01-6:	TRICHLOROETHYLENE	A-2-235
A-2-192	CAS NUMBER 75-69-4:	TRICHLOROFLUOROMETHANE (FREON 11)	A-2-236
A-2-193	CAS NUMBER 95-95-4:	TRICHLOROPHENOL, 2,4,5-	A-2-237
A-2-194	CAS NUMBER 88-06-2:	TRICHLOROPHENOL, 2,4,6-	A-2-238
A-2-195	CAS NUMBER 96-18-4:	TRICHLOROPROPANE, 1,2,3-	A-2-240
A-2-196	CAS NUMBER 108-67-8:	TRIMETHYLBENZENE, 1,3,5-	A-2-241
A-2-197	CAS NUMBER 99-35-4:	TRINITROBENZENE, 1,3,5(SYM)-	A-2-242
A-2-198	CAS NUMBER 118-96-7:	TRINITROTOLUENE, 2,4,6-	A-2-243
A-2-199	CAS NUMBER 108-05-4:	VINYL ACETATE	A-2-244
A-2-200	CAS NUMBER 75-01-4:	VINYL CHLORIDE	A-2-245
A-2-201	CAS NUMBER 108-38-3:	XYLENE, m-	A-2-246
A-2-202	CAS NUMBER 95-47-6:	XYLENE, o-	A-2-247
A-2-203	CAS NUMBER 106-42-3:	XYLENE, p-	A-2-248
A-2-204	CAS NUMBER 7440-66-6:	ZINC	A-2-249

US EPA ARCHIVE DOCUMENT

TABLE A-2-1

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).	4.13E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.84E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.22E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.90E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value calculated using K_{oc} value 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.67E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.96E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.48E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-2

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	44.05
T_m (K)	Montgomery and Welkom (1991)	149.6
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).	2.72E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.33E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	6.02E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.53E-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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.81E-02
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-3

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	179.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.99E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.04E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.88E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-05
K_{ow} (unitless)	Geometric mean value cited in Karickoff and Long (1995).	6.00E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.51E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.51E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.13E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-4

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

(Page 1 of 1)

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)	7.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.57E-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
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	4.57E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.69E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.69E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.76E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-5

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 (1995b).	5.20E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	6.10E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.03E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.73E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.37E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.69E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.69E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-6

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

(Page 1 of 1)

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 (1995b).	3.50E-01 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.10E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.34E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.92E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.22E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	9.80E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.39E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.39E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-7

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 (1995b).	1.40E-01 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	7.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.90E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.23E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.66E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.10E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-8

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)	Geometric mean value cited in U.S. EPA (1994c)	2.20E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	7.84E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.02E-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
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	1.51E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.87E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.28E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.9955

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-8a

CHEMICAL-SPECIFIC INPUTS FOR ALUMINUM (7429-90-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	26.98
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	933
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 *S* and *Vp* 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).	2.11E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in (U.S. EPA 1996a).	2.44E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (cm^3/g)	--	ND
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile (except mercury), metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-9

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 (1995b).	8.80E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.60E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	2.28E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.56E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.01E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	9.55E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.23E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.23E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.17E-01
ksg (year)$^{-1}$	NC DEHNR (1997)	3.20E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-10

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.11E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.24E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.74E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.95E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.35E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.40E+02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.50E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-11

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 (^oK)	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 (1996b), 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 same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	45 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	45 at pH=6.8
ksg $(year)^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-12

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	257.9
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.37E-07 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.71E-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.	4.23E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.69E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.43E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.53E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.32E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.32E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.29E+02
ksg (year)$^{-1}$	Mackay, Shiu, and Ma (1992).	5.06E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-13

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	327.0
T_m (K)	Montgomery and Welkom (1991)	283.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.16E-07 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.15E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.37E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.00E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.64E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.61E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.83E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.93E+03
ksg (year)$^{-1}$	Mackay, Shiu, and Ma (1992).	5.06E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	0.993

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-14

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	74.92
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,091 at 36 atm
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.07E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.24E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-15

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	215.68
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	444.1
Vp (atm)	*Vp* value cited in Budavari, O'Neil, Smith, and Heckelman (1989)	$3.66x10^{-10}$ at 25°C (solid)
S (mg/L)	*S* value cited in Howard and others 1989 - 1993	3.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.63E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.03E-06
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	4.07E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.54E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.54E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.15E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.15E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.04E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.945

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-16

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 (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-17

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	329.6
Vp (atm)	*Vp* value cited in NC DEHNR (1997).	1.30E-03 at 25ºC (solid)
S (mg/L)	*S* value cited in NC DEHNR (1997).	3.30E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.18E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.07E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.48E-06
K_{ow} (unitless)	K_{ow} value cited in NC DEHNR (1997).	3.00E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.01E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.01E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.51E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.04E-01
ksg (year)$^{-1}$	*Ksg* value assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-18

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.49E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.17E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	137
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	6.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.48E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.89E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-19

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

(Page 1 of 1)

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.28E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	3.62E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	2.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.77E+05
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	2.60E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.04E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.72E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	8.81E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-20

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

(**Page 1 of 1**)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	8.36E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	2.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	5.85E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.35E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	9.69E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.87E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	4.77E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	2.65E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-21

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	6.18E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.59E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.36E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.36E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.27E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.34E+04
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.15E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.822

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-22

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	4.15E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	1.56E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.32E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.32E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.24E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.33E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Lyman, Reehl, and Rosenblatt (1991).	1.18E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.149

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-23

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

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	122.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	395.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	8.57E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.13E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.34E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 31.98 2 31.80 3 30.13 4 19.81 5 4.81 6 0.99 7 0.55 8 0.50 9 0.50 10 0.50 11 0.50 12 0.50 13 0.50 14 0.50
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.50E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.13E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.20E-02

US EPA ARCHIVE DOCUMENT

TABLE A-2-23

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

(Page 2 of 2)

Parameter	Reference and Explanation	Value
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited Howard (1989-1993).	1.26E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-24

CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	103.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	285.85
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).	7.45E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.43E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.63E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.33E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.75E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.33E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-25

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	288.29
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	4.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.78E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.89E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.38E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	1.26E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.02E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.02E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.66E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.09E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-26

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 (1995b).	1.60E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.90E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.00E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.83E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.83E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.62E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.53E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.09E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-27

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	9.01
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,560
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.39E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.08E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-28

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.0
T_m (K)	Montgomery and Welkom (1991)	432.2
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.61E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.40E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.78E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	0.0191
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.04E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	6.30E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.76E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.76E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.32E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.05E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.87E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.000

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-29

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.83
T_m (K)	Montgomery and Welkom (1991)	582.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.45E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.42E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.46E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.9E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.40E-06
K_{ow} (unitless)	Geometric mean value cited in Karickoff and Long (1995).	6.81E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.14E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.60E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.56E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.04E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-30

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.13E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.40E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.70E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.00E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.60E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.04E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-31

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.17E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.98E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.06E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.38E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.38E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.03E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.15E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-32

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.77
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	280.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.82E-03 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.21E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.16E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.24E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.26E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.04E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-33

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 25°C (liquid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.98E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.83E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.10E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.21E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.09E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.85E+02
ksg (year)$^{-1}$	*Ksg* value wasassumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-34

CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.91E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.17E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.59E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.37E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.50E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	9.64E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-35

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.41
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	594.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.16E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.45E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-36

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.27E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.29E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.14E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.14E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.86E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.06E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-37

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.87E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.21E+02
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.52E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.08E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-38

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.64E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.37E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.66E+05
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	5.13E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.83E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.997

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-39

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.90
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	172.1
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	--	1.10E-01
D_w (cm^2/s)	--	1.27E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (mL/g)	--	ND
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-40

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 (1994b)	1.08E-05
S (mg/L)	U.S.EPA (1992a)	3.85E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.00E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.96E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.71E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.71E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.78E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.48E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Lucius (1992).	1.10E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.9999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-41

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.40E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	K_{oc} is 41 for pH range of 4.9 to 8
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.63E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due a a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-42

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	6.16E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.24E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.96E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.69E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-43

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.24E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	1.65E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	4.72E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.40E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.69E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.69E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.77E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.48E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.23E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	8.62E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-44

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

(Page 1 of 1)

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.	5.63 at 25°C (liquid)
S (mg/L)	Howard 1989-1993	2.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.68E-01
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	9.72E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.13E-05
K_{ow} (unitless)	Calculated using the log K_{ow} value cited in Howard 1989-1993.	1.20E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.83E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.38E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.93E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) OR Howard (1989-1993) OR Mackay, Shiu, and Ma (1992).	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-45

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

(Page 1 of 1)

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).	159.88 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994a)	5.74E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.80
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.53E-06
K_{ow} (unitless)	K_{ow} value calculated from log K_{ow} value cited in U.S. EPA (1995a).	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.71E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.71E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.78E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.48E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	6.72E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-46

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.03E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.17E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.09E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.90E+01
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	5.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.12E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-47

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	171.07
T_m (K)	Montgomery and Welkom (1991)	369.9
Vp (atm)	Montgomery and Welkom (1991)	7.00E-03 at 25ºC (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.70E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.04E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.38E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989 - 1993).	3.80E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.46E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.46E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.82E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-48

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	162.61
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	332.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.05E-05 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.20E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.43E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.64E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	1.17E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.14E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.36E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.86E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-49

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

(Page 1 of 2)

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 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.15E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.66E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.01E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.46E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.45E+02
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 398.0 2 398.0 3 398.0 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 (1993d) 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

US EPA ARCHIVE DOCUMENT

TABLE A-2-49

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

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	2.90E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.55E+01
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-50

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.20E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.82E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.42E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	5.85E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.40E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.40E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.55E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.96E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-51

CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	350.59
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	314.6
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-03 at 25ºC (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	5.00E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.26E-02
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.82E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.42E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.82E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.79E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.18E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-52

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	1.01E-01
D_w (cm^2/s)	D_W value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	4.63E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-53

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.0
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.58E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-54

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.21E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	6.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.48E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.97E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.97E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.23E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.19E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.53E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.761

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-54a

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	63.55
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1356.15
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 *S* and *Vp* 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).	1.19E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.38E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values estimated using the MINTEQ2 geochemical speciation model.	40 at pH=4.9 10000 at pH=6.8 28,500 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 metals, as cited in U.S. EPA (1994f).	40 at pH=4.9 10000 at pH=6.8 28,500 at pH=8.0
Kd_{bs} (cm^3/g)	Kd_{bs} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for metals, as cited in U.S. EPA (1994f).	40 at pH=4.9 10000 at pH=6.8 28,500 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because metals are nonvolatile (except mercury), they are assumed to be 100 percent in the particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

TABLE A-2-55

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 (1995b).	1.90E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.30E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.93E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	9.10E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.78E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.78E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.58E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.91E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	8.72E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-56

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	303.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.16E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.77E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.62E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.88E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.41E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.05E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.34E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.34E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.0E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.14E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-57

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

(Page 1 of 1)

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 (1995b).	1.70E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.30E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.99E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	8.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.61E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.61E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.46E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.84E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.79E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-58

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 (1995b)	177
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	6.00E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	5.60E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.29E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.50E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.83E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	4.10E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.31E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.31E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.98E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.72E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.16E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-59

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S.EPA (1992a)	26.017
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.82E-02 at 25ºC (solid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.48E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	2.10E-05
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (cm^3/g)	--	ND
ksg (year)$^{-1}$	*Ksg* value was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-60

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

(Page 1 of 1)

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.33E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.98E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.32E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.58E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.83E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.34E-02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.925

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-61

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.24E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.80E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.64E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.46E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.34E-02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.981

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-62

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.37E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.48E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.17E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.78E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.71E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.34E-02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.852

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-63

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	278.34
T_m (K)	Montgomery and Welkom (1991)	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.55E-08 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.08E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.43E-06
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.38E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.86E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.25E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.57E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.27E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.11E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.989

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-64

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (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).	5.88E-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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.65E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.14E+09
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.03E+08
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.03E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.78E+07
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.61E+07
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.9081

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-65

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)	304.36
T_m (K)	Howard (1989-1993)	393.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.11E-07 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	6.88E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.89E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.71E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.33E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.33E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.96E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.31E+01
ksg (year)$^{-1}$	--	ND
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-66

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	539.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.70E-14 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.70E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.12E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.53E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.79E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.16E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.69E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.011

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-67

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 (1995b).	1.0E-03 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.97E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.79E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.79E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.19E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.47E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.47E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.10E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.79E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-68

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

(Page 1 of 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 (1995b).	3.44E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.21E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.96E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	1.50E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.05E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.05E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.29E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.82E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-69

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.11E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.93E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.79E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.79E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay and others (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii

US EPA ARCHIVE DOCUMENT

TABLE A-2-70

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	297.86
Vp (atm)	*Vp* value cited in Howard (1989-1993).	3.03E-03 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	6.88E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S,* and *Vp* values that are provided in this table.	1.11E+02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.85E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.39E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.03E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.03E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.02E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.21E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-71

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.80E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.85E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.58E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.16E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.46E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-72

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.08E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.48E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.76E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.70E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.70E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.52E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.48E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	0.847

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-73

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 (1995b).	6.40E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.0E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.58E+00
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.77E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.00E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.44E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.85E+0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.85E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.14E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.74E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-74

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	98.97
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	175.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.0E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.16E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.75E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.42E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	6.20E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	5.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.12E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.643
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-75

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.27E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.90E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.96E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.83E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-76

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	150.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.88E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.0E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.55E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.53E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.09E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.32E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.88E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.60E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-77

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.51E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.13E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.60E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.98E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.98E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.73+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.99E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-78

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.44E-03
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.16E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	9.75E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	9.60E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.80E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-79

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	163.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	318.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.21E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.93E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.38E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.79E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.09E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 159.0 2 159.0 3 159.0 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 2.40 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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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

US EPA ARCHIVE DOCUMENT

TABLE A-2-79

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

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.58E+00
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-80

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.71E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.88E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.96E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-81

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	Montgomery and Welkom (1991)	189.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.11E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.55E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.94E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.26E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	5.60E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.08E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.24E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-82

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	220.98
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in Howard (1989-1993).	6.93E-05 at 25ºC (liquid)
S (mg/L)	*S* value cited in Howard (1989-1993).	1.6E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.57E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.33E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.69E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.85E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.85E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.38E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.38E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.49E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-83

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

(Page 1 of 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)	Geometric mean value cited in U.S. EPA (1994c)	1.31E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.87E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.66E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.29E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.86E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.55E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.02E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	2.34E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.9860

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-84

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.48E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.73E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.28E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.52E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-85

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.01E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.96E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.13E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.30E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.09E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.09E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.00E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.06E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-86

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

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Moses (1978)	122.17
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	300.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.66E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	6.25E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.24E-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
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.29E+02
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 126.0 2 126.0 3 126.0 4 126.0 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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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

US EPA ARCHIVE DOCUMENT

TABLE A-2-86

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

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.04E+00
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-87

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 (1995b).	3.30E-10 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.40E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.36E-10
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.38E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	5.60E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.46E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.65E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.65E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.74E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.46E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.877

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-88

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	168.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	363
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f).	4.0E-07 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	5.4E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.25E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	3.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	9.15E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	3.10E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.06E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.06E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.55E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.25E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-89

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

(Page 1 of 2)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.82E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.06E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.30E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 0.80 2 0.79 3 0.72 4 0.38 5 0.08 6 0.02 7 0.01 8 0.01 9 0.01 10 0.01 11 0.01 12 0.01 13 0.01 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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value calculated 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	7.5E-04 (at pH 7.0)
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	4.0E-04 (at pH 7.0)

US EPA ARCHIVE DOCUMENT

TABLE A-2-89

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

Parameter	Reference and Explanation	Value
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.62E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-90

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.85E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.46E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.86E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.90E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.10E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.83E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.04E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.999

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-91

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 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.05E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.30E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.19E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.19E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.14E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.68E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-92

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 (1995b)	5.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	9.00E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.89E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.20E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	5.40E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.76E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.76E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.57E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.50E-02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-93

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 (1995b)	4.74E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	6.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.28E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.95E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	8.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.78E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.78E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.09E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.11E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.999

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-94

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 (1995b).	248
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.7E-07 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.6E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.12E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.21E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	9.55E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.20E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.20E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.998

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-95

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

(Page 1 of 1)

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)	Geometric mean value cited in U.S. EPA (1994c)	1.31E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.31E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.31E-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
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.02E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.16E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.78E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9839

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-96

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.19E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.07E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.79E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.08E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.11E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.32E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	3.61E+04
Fv (unitless)	--	ND

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-97

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (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 (1995b).	2.20E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	6.60E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.08E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.13E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.66E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.88E-02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-98

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 (1995b)	114.14
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.30E-02 at 25ºC
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.38E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.07E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.35E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.89E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.46E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.85E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.80E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value cited in NC DEHNR (1997).	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-99

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

(Page 1 of 1)

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 (1995b).	3.50E-04 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.90E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.87E-08
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.63E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.84E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.12E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.55E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.55E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.16E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.19E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.88E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-100

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.73E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.33E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.16E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	2.53E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-101

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 (1995b).	1.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.47E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.17E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.19E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	5.62E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.28E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.28E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.46E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.31E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-102

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	44.05
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	162.1
Vp (atm)	Verschueren (1983)	1.44E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in NC DEHNR (1996).	3.80E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.67E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.71E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.44E-05
K_{ow} (unitless)	Howard (1989-1993)	5.01E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	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 (1993d) 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-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.19E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.30E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.13E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-103

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 (1994c).	8.49E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.96E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.37E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.22E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.60E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1994c).	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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.33E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.44E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.10E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.9350

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-104

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	383.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.07E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.32E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.33E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.75E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.18E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.21E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.91E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.96E+03
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	5.75E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.992

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-105

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)	Geometric mean value cited in U.S. EPA (1994c)	8.17E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.86E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.30E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	3.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	7.88E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	1.47E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.71E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.08E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.22E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-106

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 (1995b)	5.50E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.78E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.00E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.74E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	2.20E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.62E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.62E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.96E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.05E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-107

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995b)	46.03
T_m (K)	U.S. EPA (1995b)	282.0
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	5.40E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.00E+06
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.49E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.22E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.71E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	2.90E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.39E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.39E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.04E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.16E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-108

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	425.31
T_m (K)	U.S. EPA (1994a)	537.1
Vp (atm)	U.S. EPA (1994a)	4.22E-14 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	2.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	7.50E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.11E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.89E-06
K_{ow} (unitless)	U.S. EPA (1992d)	1.58E+08
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	9.77E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.77E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.33E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.91E+06
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.62E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-109

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	409.31
T_m (K)	U.S. EPA (1994a)	509.1
Vp (atm)	U.S. EPA (1994a)	1.75E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	1.35E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	5.30E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.55E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.99E-06
K_{ow} (unitless)	U.S. EPA (1992d)	8.32E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+06
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	3.47E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-110

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	409.31
T_m (K)	U.S. EPA (1994a)	494.1
Vp (atm)	U.S. EPA (1994a)	1.41E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	5.30E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.55E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.99E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	8.32E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+06
ksg (year)$^{-1}$	*ksg* value was calculated using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	2.01E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-111

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	373.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.73E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.87E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.69E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.04E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.53E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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. 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.81E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-112

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

(Page 1 of 1)

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)	Geometric mean value cited in U.S. EPA (1994c)	5.71E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.68E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.29E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.62E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.18E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.18E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.38E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.87E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.58E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9948

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-113

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	546.1
Vp (atm)	U.S. EPA (1994a)	1.33E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	4.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	U.S. EPA (1992d)	6.17E+07
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; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.80E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+06
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	5.96E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-114

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	558.1
Vp (atm)	U.S. EPA (1994a)	4.74E-14 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	4.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDD.	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*ksg* value assumed to be the same as the *ksg* value calculated for 1,2,3,4,7,8-HexaCDD. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	2.89E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-115

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	516.1
Vp (atm)	U.S. EPA (1994a)	6.45E-14 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	4.40E-06
H (atm·m^3/mol)	U.S.EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1994a).	1.78E+07
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; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*ksg* value was assumed to be the same as the *ksg* value for 1,2,3,4,7,8-HexaCDD. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.53E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-116

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	498.6
Vp (atm)	U.S. EPA (1994a)	3.16E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	8.25E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.40E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d)	1.78E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	4.86E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-117

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	505.1
Vp (atm)	U.S. EPA (1994a)	2.89E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	1.77E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	6.10E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue groupaverage value obtained from U.S. EPA (1992d)	1.78E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	5.15E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-118

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	519.1
Vp (atm)	U.S. EPA (1994a)	2.37E-13 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.30E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.00E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.5759

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-119

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	512.1
Vp (atm)	U.S. EPA (1994a)	2.63E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.30E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.00E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	5.47E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-120

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 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.54E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.33E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.38E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.94E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.94E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.20E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.77E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-121

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	5.35E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.84E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.18E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.00E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.20E+03
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.21E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-122

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.72E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.07E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.51E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.51E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.13E+2
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.80E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-123

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.60E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.77E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.88E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.66E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.82E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.82E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.36E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.27E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-124

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 (1995b).	3.60E-15 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.0E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.88E-10
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.46E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.01E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.47E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.08E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.08E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.08E+04
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.31E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.71E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.4E-04

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-125

CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	36.47
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	158.9
Vp (atm)	U.S. EPA (1994b)	4.6E+01 (liquid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.73E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	2.00E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (mL/g)	--	ND
ksg (year)$^{-1}$	--	ND
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-126

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	4.86E-09
D_a (cm^2/s)	D_a value was obtained from WATER8 model database U.S. EPA (1995d)	1.90E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database U.S. EPA (1995d)	5.66E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	8.22E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.11E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.11E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.08E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.64E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.47E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.007

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-127

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)	Geometric mean value cited in U.S. EPA (1994c)	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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.20E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.22E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.50E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.00E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.99E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.99E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.25E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.20E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-128

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	207.2
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	600.5
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.43E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.28E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from Baes, Sharp, Sjoreen, and Shor (1984), which states that several factors, such as experimental methods and soil type, could influence partitioning or Kd_s values. Baes, Sharp, Sjoreen, and Shor (1984) compares values between various literature sources and provide this value, which is based on its best judgment.	9.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	9.00E+02
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	9.00E+02
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-129

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	330.36
T_m (K)	Montgomery and Welkom (1991)	276
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.04E-08 at 25°C (liquid)
S (mg/L)	*S* value cited in Howard (1989-1993).	1.43E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.40E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.29E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.29E+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.	9.81E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.81E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.36E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.92E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	0.946

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-130

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	271.52
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	550.1
Vp (atm)	U.S. EPA (1996a)	1.20E-04
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	6.90E+04
H (atm·m^3/mol)	U.S. EPA (1997g)	7.1E-10
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	4.53E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.25E-06
K_{ow} (unitless)	U.S. EPA (1996a)	6.10E-01
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S. EPA (1997g)	5.80E+04
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	1.00E+05
Kd_{bs} (mL/g)	U.S. EPA (1997g)	5.00E+04
ksg (year)$^{-1}$	U.S. EPA (1996a)	0.0
Fv (unitless)	Estimated based on discussions concerning divalent mercury provided in U.S. EPA (1996a).	0.85

Note:
NA = Not Applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-131

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	200.59
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	234.23
Vp (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	2.63E-06 at 25°C
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	5.62E-02
H (atm·m^3/mol)	U.S. EPA (1997g)	7.1E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_a values. A density value of 13.546 g/cc for mercury was used.	1.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_w values. A density value of 13.546 g/cc for mercury was used.	3.01E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S.EPA (1997g)	1.00E+03
Kd_{sw} (L/Kg)	U.S.EPA (1997g)	1.00E+03
Kd_{bs} (mL/g)	U.S.EPA (1997g)	3.00E+03
ksg (yr)$^{-1}$	U.S. EPA (1996a)	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not available
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-132

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 (1995b)	8.90E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.15E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.33E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	3.47E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.74E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.74E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.80E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.49E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-133

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

(Page 1 of 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 (1995b)	2.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.44E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.64E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	1.95E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.96E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.96E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.97E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.58E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-134

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.33E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.59E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.36E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.00E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.20E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	6.93E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.901

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-135

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	74.08
T_m (K)	Montgomery and Welkom (1991)	175.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	2.84E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.44E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.64E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.23E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.90E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.25E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.25E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.44E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.30E-01
ksg (year)$^{-1}$	*Ksg* value assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-136

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.41E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.21E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.30E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.60E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

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Note
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-137

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.52E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.13E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.39E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.00E+00
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.40E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boehling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-138

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 (1995b).	1.20E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.40E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.61E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.35E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.91E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.34E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.34E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.76E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.36E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-139

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

(Page 1 of 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 (1995b).	2.50E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.25E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.59E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.36E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.55E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.00E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.80E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-140

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1997g)	216.0
T_m (^oK)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	U.S. EPA (1997g)	4.7E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	5.28E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.11E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	U.S. EPA (1997g)	7.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	1.00E+05
Kd_{bs} (mL/g)	U.S. EPA (1997g)	3.00E+03
ksg $(year)^{-1}$	U.S. EPA (1996a)	0.0
Fv (unitless)	Based on discussions provided in U.S. EPA (1996a), methyl mercury does not exist in the air/vapor phase.	0.0

Note:
NA = Not Applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-141

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	7.20E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.59E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.966

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-142

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	173.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	220.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.20E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.45E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.64E-02
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.10E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.60E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.04E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-143

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	84.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.87E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	8.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	1.25E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.00E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.00E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.50E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.00E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-144

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

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	128.16
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	353.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.17E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.11E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.82E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.26E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.92E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.36E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.19E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.93E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.76E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.27E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-145

NICKEL (7440-02-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.69
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,828
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.26E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.46E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-146

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	342.1
Vp (atm)	*Vp* value cited in Montgomery and Welcom (1991).	1.07E-05 at 25°C (solid)
S (mg/L)	*S* value cited in Montgomery and Welcom (1991).	1.26E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.29E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.81E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	7.08E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.93E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.93E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.95E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+00
ksg (year)$^{-1}$	*Ksg* value wasassumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-147

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

(Page 1 of 1)

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
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.34E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.66E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.62E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-148

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	419.10
Vp (atm)	--	ND
S (mg/L)	*S* value cited in Montgomery and Welcom (1991)	1.07E-05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	1.65E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.31E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.46E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.72E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.89E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-149

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	2.06E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	9.43E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	6.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.19E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.93E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.76E+004
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.28E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the liquid-phase *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-150

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

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.46E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.44E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.19E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.53E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.53E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.65E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.41E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-151

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

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	386.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-06 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.32E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.61E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	8.13E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.37E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.37E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.28E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.75E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.09E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-152

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 (1995b)	158.20
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	3.80E-04 at 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.47E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.52E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	2.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.07E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.07E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.29E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.44E+00
Fv (unitless)	*Fv* value cited in NC DEHNR (1997).	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

(Page 1 of 1)

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)	Geometric mean value cited in U.S. EPA (1994c)	1.32E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	3.74E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.99E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.06E+03
K_{oc} (mL/g)	Estimated value was obtained from U.S. EPA (1994c).	3.27E+02, for pH range of 4.9 to 8.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.31E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.44E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	130.19
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.63E-03 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.46E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.67E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.75E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	2.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.28E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.80E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	460.76
T_m (K)	U.S. EPA (1994a)	598.1
Vp (atm)	U.S. EPA (1994a)	1.09E-15 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	7.40E-08
H (atm·m^3/mol)	U.S. EPA (1994a)	7.00E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.69E-07
K_{ow} (unitless)	U.S. EPA (1994a)	3.89E+07
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; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.40E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.60E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.0017

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	444.76
T_m (K)	U.S. EPA (1994a)	531.1
Vp (atm)	U.S. EPA (1994a)	4.93E-15 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	1.20E-06
H (atm·m^3/mol)	U.S.EPA (1994a)	1.90E-06
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 calculated using the equation cited in U.S. EPA (1996a).	3.78E-06
K_{ow} (unitless)	U.S. EPA (1994a)	6.03E+08
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) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.72E+08
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.72E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.79E+07
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.49E+07
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.10E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.67E-03

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-157

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	356.42
T_m (K)	U.S. EPA (1994a)	513.1
Vp (atm)	U.S. EPA (1994a)	1.25E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.20E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	2.60E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.21E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.38E-06
K_{ow} (unitless)	U.S. EPA (1992d)	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.69E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.08E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	2.19E-01

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	340.42
T_m (K)	U.S. EPA (1994a)	498.1
Vp (atm)	U.S. EPA (1994a)	3.58E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	2.40E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	6.17E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.80E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+05
ksg (year)$^{-1}$	*ksg* value assumed to be the same as the *ksg* value calculated for 2,3,4,7,8-PentaCDF. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	3.64E-01

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

TABLE A-2-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	340.42
T_m (K)	U.S. EPA (1994a)	469.1
Vp (atm)	U.S. EPA (1994a)	4.33E-12 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	2.36E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	8.32E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	2.63E-01

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.43E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.86E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.34E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.22E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.21E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.41E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.29E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.33E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-161

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)	3.1E-06 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	2.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	5.0E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	4.37E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.89E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.42E+02
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.36E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.62E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	266.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	463
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.11E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.34E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.41E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	8.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+05
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 / 19,949 2 / 19,918 3 / 19,604 4 / 16,942 5 / 7,333 6 / 1,417 7 / 504.9 8 / 408.7 9 / 399.1 10 / 398.1 11 / 398.0 12 / 398.0 13 / 398.0 14 / 398.0
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	pH / K_{oc} 1 / 199.5 2 / 199.2 3 / 196.0 4 / 169.4 5 / 73.33 6 / 14.17 7 / 5.05 8 / 4.09 9 / 3.99 10 / 3.98 11 / 3.98 12 / 3.98 13 / 3.98 14 / 3.98

US EPA ARCHIVE DOCUMENT

TABLE A-2-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(**Page 2 of 2**)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	pH / K_{oc} 1 / 1,496 2 / 1,494 3 / 1,470 4 / 1,271 5 / 550.0 6 / 106.2 7 / 37.87 8 / 30.66 9 / 29.93 10 / 29.86 11 / 29.85 12 / 29.85 13 / 29.85 14 / 29.85
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	pH / K_{oc} 1 / 798.0 2 / 796.7 3 / 784.1 4 / 677.7 5 / 293.3 6 / 56.67 7 / 20.20 8 / 16.35 9 / 15.96 10 / 15.92 11 / 15.92 12 / 15.92 13 / 15.92 14 / 15.92
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.42E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in of LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-163

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 25ºC (solid)
S (mg/L)	*S* value cited in Lucius et al. (1992).	1.28E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.88E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.33E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.47E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.55E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.09E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.09E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.35E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.26E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	94.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	314.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.74E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	9.08E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.95E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	3.00E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 22.0 2 22.0 3 22.0 4 22.0 5 22.0 6 22.0 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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.79E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.53E+01

US EPA ARCHIVE DOCUMENT

TABLE A-2-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-165

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 (1995b).	3.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.16E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.05E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.88E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.33E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.33E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.96E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.31E+01
ksg (year)$^{-1}$	*Ksg value* was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	148.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	403.9
Vp (atm)	Howard (1989-1993)	2.63E-07 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	6.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.28E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.04E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.97E-06
K_{ow} (unitless)	NC DEHNR (1997)	2.5E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.10E-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 (1993d) 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.	2.10E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.40E-03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.35E+04
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-167

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

(Page 1 of 1)

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 (1995b)	5.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.50E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.05E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.71E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.45E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	3.24E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.74E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.74E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.81E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.10E+01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-168

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 (1994c).	5.59E-09 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.37E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.25E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.80E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.72E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992)	1.33E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9946

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-169

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

(Page 1 of 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 (1995b)	2.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	3.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.86E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.08E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	4.68E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.72E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.72E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.54E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.89E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-170

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	321.57
T_m (K)	Montgomery and Welkom (1991)	314.1
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.05E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.69E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.17E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.28E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.28E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.56E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.10E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-171

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 (1995b).	1.10E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.50E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.19E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.06E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.16E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.68E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.68E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.26E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.73E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.96
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.03E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.20E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)		NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.87
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.38E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.71E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

(Page 1 of 1)

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 (1995b).	2.20E-13 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.50E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.90E-13
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.38E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.58E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	8.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.53E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.53E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.81E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using S, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.086

Note:
NA = Note applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-175

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	104.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	8.21E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.57E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.33E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.49E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.12E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.65E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-176

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)	U.S. EPA (1994a)	1.60E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.81E-06
K_{ow} (unitless)	U.S. EPA (1994a)	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.69E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.08E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	4.29E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.4901

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-177

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	305.98
T_m (K)	U.S. EPA (1994a)	500.1
Vp (atm)	U.S. EPA (1994a)	1.17E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	4.19E-04
H (atm·m^3/mol)	U.S. EPA (1994a).	8.60E-06
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	1.79E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.85E-06
K_{ow} (unitless)	U.S. EPA (1992d)	3.39E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.09E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.09E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.36E+04
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.6634

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-178

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 (1995b).	7.1E-06 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.18E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.36E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.89E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.42E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.36E+02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

(Page 1 of 1)

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 (1995b)	1.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.44E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	4.27E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.59E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.59E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.37E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.75E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-180

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.72E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.26E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.40E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.90E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.93E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.16E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.75E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-181

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

(Page 1 of 1)

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.73E-02
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	7.20E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	3.51E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.65E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.06E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-182

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 (1995b)	231.89
T_m (K)	U.S. EPA (1995b)	343.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.60E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.53E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.55E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	5.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.0E+04
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 / 6,190 2 / 6,188 3 / 6,166 4 / 5,956 5 / 4,456 6 / 1,323 7 / 249.2 8 / 115.3 9 / 101.6 10 / 100.2 11 / 100.0 12 / 100.0 13 / 100.0 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 (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	18.69
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	9.97
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41

US EPA ARCHIVE DOCUMENT

TABLE A-2-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	72.1
T_m (K)	Montgomery and Welkom (1991)	164.6
Vp (atm)	*Vp* value cited in Budavari, O'Neil, Smith, and Heckleman (1989).	2.14E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994b).	1.00E+06
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.54E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.31E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.07E-05
K_{ow} (unitless)	Value cited in Karickoff and Long (1995).	2.80E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.16E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.26E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	4.43E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	204.38
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.34E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	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 same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-185

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	92.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.71E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.58E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.13E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	4.65E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.60E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	1.15E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-186

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 (1995b).	3.94E-04 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.43E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.12E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.19E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.57E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.18E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.28E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-187

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

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)	325.7
Vp (atm)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	3.20E-04 at 25°C (solid)
S (mg/L)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	2.05E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.84E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.02E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.15E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.11E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.02E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.10E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-188

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.61E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	9.73E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.66E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.64E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-189

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.17E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.66E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.56E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.64E+02
K_{oc} (mL/g)	Geometric mean value cited in U.S. EPA (1996b)	1.35E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the 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+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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+04
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.40E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.26E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-190

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)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.25E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.63E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.00E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	6.93E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-191

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	131.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	188.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.48E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.18E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.06E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.94E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.40E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.40E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.76E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	0.703
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-192

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

(Page 1 of 1)

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 (1995b).	1.10E+00 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.37E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	3.40E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.34E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.34E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.00E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.34E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-193

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 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.64E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.91E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.03E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.41E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 2,380 2 2,380 3 2,380 4 2,377 5 2,353 6 2,139 7 1,127 8 223.7 9 56.14 10 37.94
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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. Kd_s value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	1.13E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	8.45E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Kd_{bs} value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	4.51E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	0.367
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	197.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	342.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.55E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.06E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.08E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.15E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 / 1,070 2 / 1,070 3 / 1,069 4 / 1,063 5 / 1,006 6 / 670.8 7 / 226.2 8 / 120.4 9 / 108.4 10 / 107.1
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) 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. Kd_s value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	2.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.70E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	9.05E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+00

US EPA ARCHIVE DOCUMENT

TABLE A-2-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-195

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 (1995b).	4.90E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.80E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.99E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.05E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.04E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.22E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.19
T_m (K)	Montgomery and Welkom (1991)	287.9
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	2.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.86E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989-1993).	2.63E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.67E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.67E+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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.25E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.69E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.16E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-197

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 (1995b).	1.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.20E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.66E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.84E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	6.08E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.18E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.18E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.84E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.72E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-198

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)	Value cited in U.S. EPA (1994b).	2.63E-07
S (mg/L)	Value cited in U.S. EPA (1994b).	1.30E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.59E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	3.98E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.51E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.51E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.88E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.00E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	1.41E+00
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	0.9980

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-199

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	86.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	180.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.43E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.24E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.50E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.94E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.00E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.97E+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 (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.97E-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 (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.99E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-200

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	62.50
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	119.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.68E+00 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.15E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.19E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.11E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.11E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction 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-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.44E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (108-38-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	225.7
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.86E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.49E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.59E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.96E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.96E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.47E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.84E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.000

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (95-47-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	248.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.86E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.44E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.35E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.41E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.41E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.81E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.64E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.000

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (106-42-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	286.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.86E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.61E+02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.50E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.48E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.11E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.11E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.33E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.24E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

US EPA ARCHIVE DOCUMENT

TABLE A-2-204

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 (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	692.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989)	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.17E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), 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 same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	6.2E+01 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	6.2E+01 at pH=6.8
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

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

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

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