Appendix B

Physical-Chemical Properties for Chemicals Included in IWAIR

Appendix B

Physical-Chemical Properties for Chemicals Included in IWAIR

This appendix presents the physical-chemical property values included in IWAIR and the sources of those values. Each table provides the data for one chemical; the chemicals are shown in CAS-number order. The following source references are used throughout:

Calculated based on EPA (1987)	U.S. EPA (1987)
Calculated based on Lyman (1990)	Lyman et al. (1990)
Calculated based on WATER9 (2001)	U.S. EPA (2001)
Calculated based on EPA's Dioxin Reassessment (2000)	U.S. EPA (2000)
CHEMDAT8	U.S. EPA (1994)
Chemfate	SRC (2000)
ChemFinder	CambridgeSoft (2001)
Dioxin Reassessment	U.S. EPA (2000)
Hansch et al. (1995) (unpub)	Hansch et al. (1995)
Howard et al. (1991)	Howard et al. (1991)
HSDB	U.S. NLM (2001)
Kollig (1993)	Kollig (1993)
KowWIN	SRC (2001)
Mackay et al. (1992)	Mackay et al. (1992)
Merck	Budavari (1996)
MRTC	U.S. EPA (1997a)
SCDM	U.S. EPA (1997b)

Table B-1. Chemical-Specific Inputs for Formaldehyde (50-00-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.1E-01	g/cm3	SCDM
HLC	Henry's law constant	3.4E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-5.0E-02	unitless	SCDM
MW	Molecular Weight	3.0E+01	g/mol	SCDM
Sol	Solubility	5.5E+05	mg/L	SCDM
VP	Vapor pressure	5.2E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	5.0E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.7E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.7E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.7E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-2. Chemical-Specific Inputs for Benzo(a)pyrene (50-32-8)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	1.1E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.1E+00	unitless	SCDM
MW	Molecular Weight	2.5E+02	g/mol	SCDM
Sol	Solubility	1.6E-03	mg/L	SCDM
VP	Vapor pressure	5.5E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	1.4E+00	g/cm3	HSDB
Ksg	Soil degradation rate	1.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	9.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	6.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-3. Chemical-Specific Inputs for N-Nitrosodiethylamine (55-18-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.4E-01	g/cm3	SCDM
HLC	Henry's law constant	3.6E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.8E-01	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	9.3E+04	mg/L	SCDM
VP	Vapor pressure	8.6E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.4E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-4. Chemical-Specific Inputs for Carbon tetrachloride (56-23-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	3.0E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.7E+00	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	7.9E+02	mg/L	SCDM
VP	Vapor pressure	1.2E+02	mmHg	SCDM
Kh	Hydrolysis rate	5.4E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.5E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-5. Chemical-Specific Inputs for 3-Methylcholanthrene (56-49-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	9.4E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.4E+00	unitless	SCDM
MW	Molecular Weight	2.7E+02	g/mol	SCDM
Sol	Solubility	3.2E-03	mg/L	SCDM
VP	Vapor pressure	7.7E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.7E-09	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	6.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-6. Chemical-Specific Inputs for 7,12-Dimethylbenz[a]anthracene (57-97-6)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.1E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.6E+00	unitless	SCDM
MW	Molecular Weight	2.6E+02	g/mol	SCDM
Sol	Solubility	2.5E-02	mg/L	SCDM
VP	Vapor pressure	5.6E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.7E-02	cm2/s	Calculated based on EPA, 1987.
Dw	Diffusion coefficient in water	5.5E-06	cm2/s	Calculated based on EPA, 1987.
Density	Density of the chemical	1.0E+00	g/cm3	-

Table B-7. Chemical-Specific Inputs for Aniline (62-53-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	1.9E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	9.8E-01	unitless	SCDM
MW	Molecular Weight	9.3E+01	g/mol	SCDM
Sol	Solubility	3.6E+04	mg/L	SCDM
VP	Vapor pressure	4.9E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.6E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.1E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	7.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-8. Chemical-Specific Inputs for Methanol (67-56-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.9E-01	g/cm3	SCDM
HLC	Henry's law constant	4.5E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-7.1E-01	unitless	SCDM
MW	Molecular Weight	3.2E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	1.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.6E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.7E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-9. Chemical-Specific Inputs for Acetone (67-64-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.9E-01	g/cm3	SCDM
HLC	Henry's law constant	3.9E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-2.4E-01	unitless	SCDM
MW	Molecular Weight	5.8E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	2.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.1E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.3E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-10. Chemical-Specific Inputs for Chloroform (67-66-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	3.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.9E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	7.9E+03	mg/L	SCDM
VP	Vapor pressure	2.0E+02	mmHg	SCDM
Kh	Hydrolysis rate	3.2E-12	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.3E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-11. Chemical-Specific Inputs for Hexachloroethane (67-72-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.1E+00	g/cm3	SCDM
HLC	Henry's law constant	3.9E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.0E+00	unitless	SCDM
MW	Molecular Weight	2.4E+02	g/mol	SCDM
Sol	Solubility	5.0E+01	mg/L	SCDM
VP	Vapor pressure	2.1E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-12. Chemical-Specific Inputs for N,N-Dimethyl formamide (68-12-2)

Parameter	Definition	Value	Units	Reference
Ksg	Soil degradation rate	1.0E-20	sec-1	no value for Ksg in existing hierarchy
Density	Density of the chemical	9.4E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
HLC	Henry's law constant	7.4E-08	atm-m3/mol	HSDB
Sol	Solubility	1.0E+06	mg/L	HSDB
VP	Vapor pressure	3.7E+00	mmHg	HSDB
LogKow	Octanol-water partition coeficient	-1.0E+00	unitless	Hansch et al., 1995
MW	Molecular Weight	7.3E+01	g/mol	Chemfate
K1	Aqueous degradation rate (low)	1.3E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-13. Chemical-Specific Inputs for Benzene (71-43-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.8E-01	g/cm3	SCDM
HLC	Henry's law constant	5.6E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	7.8E+01	g/mol	SCDM
Sol	Solubility	1.8E+03	mg/L	SCDM
VP	Vapor pressure	9.5E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.9E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-14. Chemical-Specific Inputs for 1,1,1-Trichloroethane (71-55-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	1.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	1.3E+03	mg/L	SCDM
VP	Vapor pressure	1.2E+02	mmHg	SCDM
Kh	Hydrolysis rate	2.0E-08	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-15. Chemical-Specific Inputs for Methyl bromide (74-83-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.7E+00	g/cm3	SCDM
HLC	Henry's law constant	6.2E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.2E+00	unitless	SCDM
MW	Molecular Weight	9.5E+01	g/mol	SCDM
Sol	Solubility	1.5E+04	mg/L	SCDM
VP	Vapor pressure	1.6E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-16. Chemical-Specific Inputs for Methyl chloride (74-87-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.1E-01	g/cm3	SCDM
HLC	Henry's law constant	8.8E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	9.1E-01	unitless	SCDM
MW	Molecular Weight	5.0E+01	g/mol	SCDM
Sol	Solubility	5.3E+03	mg/L	SCDM
VP	Vapor pressure	4.3E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.2E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.5E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.2E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.4E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-17. Chemical-Specific Inputs for Vinyl chloride (75-01-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.1E-01	g/cm3	SCDM
HLC	Henry's law constant	2.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	6.3E+01	g/mol	SCDM
Sol	Solubility	2.8E+03	mg/L	SCDM
VP	Vapor pressure	3.0E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.7E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-18. Chemical-Specific Inputs for Acetonitrile (75-05-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.9E-01	g/cm3	SCDM
HLC	Henry's law constant	3.5E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-3.4E-01	unitless	SCDM
MW	Molecular Weight	4.1E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.1E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.3E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.4E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-19. Chemical-Specific Inputs for Acetaldehyde (75-07-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.8E-01	g/cm3	SCDM
HLC	Henry's law constant	7.9E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-4.7E-01	unitless	SCDM
MW	Molecular Weight	4.4E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.0E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	8.2E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.6E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.3E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-20. Chemical-Specific Inputs for Methylene chloride (75-09-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	2.2E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.3E+00	unitless	SCDM
MW	Molecular Weight	8.5E+01	g/mol	SCDM
Sol	Solubility	1.3E+04	mg/L	SCDM
VP	Vapor pressure	4.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-21. Chemical-Specific Inputs for Carbon disulfide (75-15-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	3.0E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	7.6E+01	g/mol	SCDM
Sol	Solubility	1.2E+03	mg/L	SCDM
VP	Vapor pressure	3.6E+02	mmHg	SCDM
Ksg	Soil degradation rate	1.0E-20	sec-1	no value for Ksg in existing hierarchy
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
K1	Aqueous degradation rate (low)	8.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-22. Chemical-Specific Inputs for Ethylene oxide (75-21-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.9E-01	g/cm3	Merck
Kh	Hydrolysis rate	6.7E-07	sec-1	Kollig, 1993
Sol	Solubility	1.0E+06	mg/L	HSDB
Ksg	Soil degradation rate	6.8E-07	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	-3.0E-01	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.5E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	4.4E+01	g/mol	Chemfate
VP	Vapor pressure	1.3E+03	mmHg	Chemfate
K1	Aqueous degradation rate (low)	9.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.3E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.5E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-23. Chemical-Specific Inputs for Tribromomethane (75-25-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.9E+00	g/cm3	SCDM
HLC	Henry's law constant	5.3E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.4E+00	unitless	SCDM
MW	Molecular Weight	2.5E+02	g/mol	SCDM
Sol	Solubility	3.1E+03	mg/L	SCDM
VP	Vapor pressure	5.5E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-24. Chemical-Specific Inputs for Bromodichloromethane (75-27-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.0E+00	g/cm3	SCDM
HLC	Henry's law constant	1.6E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	1.6E+02	g/mol	SCDM
Sol	Solubility	6.7E+03	mg/L	SCDM
VP	Vapor pressure	5.0E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-25. Chemical-Specific Inputs for 1,1-Dichloroethylene (75-35-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.6E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	9.7E+01	g/mol	SCDM
Sol	Solubility	2.3E+03	mg/L	SCDM
VP	Vapor pressure	6.0E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	9.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-26. Chemical-Specific Inputs for Propylene oxide (75-56-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.6E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
VP	Vapor pressure	5.4E+02	mmHg	HSDB
Ksg	Soil degradation rate	6.5E-07	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	3.0E-02	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.2E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	5.8E+01	g/mol	Chemfate
Sol	Solubility	4.1E+05	mg/L	Chemfate
K1	Aqueous degradation rate (low)	1.7E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-27. Chemical-Specific Inputs for Trichlorofluoromethane (75-69-4)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	9.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E+00	unitless	SCDM
MW	Molecular Weight	1.4E+02	g/mol	SCDM
Sol	Solubility	1.1E+03	mg/L	SCDM
VP	Vapor pressure	8.0E+02	mmHg	SCDM
Density	Density of the chemical	1.5E+00	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.2E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-28. Chemical-Specific Inputs for Dichlorodifluoromethane (75-71-8)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.4E-01	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.2E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	2.8E+02	mg/L	SCDM
VP	Vapor pressure	4.8E+03	mmHg	SCDM
Density	Density of the chemical	1.5E+00	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.7E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-29. Chemical-Specific Inputs for 1,1,2-Trichloro-1,2,2-trifluoroethane (76-13-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	4.8E-01	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.2E+00	unitless	SCDM
MW	Molecular Weight	1.9E+02	g/mol	SCDM
Sol	Solubility	1.7E+02	mg/L	SCDM
VP	Vapor pressure	3.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-30. Chemical-Specific Inputs for Hexachlorocyclopentadiene (77-47-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.7E+00	g/cm3	SCDM
HLC	Henry's law constant	2.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	5.4E+00	unitless	SCDM
MW	Molecular Weight	2.7E+02	g/mol	SCDM
Sol	Solubility	1.8E+00	mg/L	SCDM
VP	Vapor pressure	6.0E-02	mmHg	SCDM
Kh	Hydrolysis rate	7.9E-07	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.4E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-31. Chemical-Specific Inputs for Isophorone (78-59-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.3E-01	g/cm3	SCDM
HLC	Henry's law constant	6.6E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.7E+00	unitless	SCDM
MW	Molecular Weight	1.4E+02	g/mol	SCDM
Sol	Solubility	1.2E+04	mg/L	SCDM
VP	Vapor pressure	4.4E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-32. Chemical-Specific Inputs for 1,2-Dichloropropane (78-87-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.8E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.8E+03	mg/L	SCDM
VP	Vapor pressure	5.2E+01	mmHg	SCDM
Kh	Hydrolysis rate	1.5E-09	sec-1	Kollig, 1993
Ksg	Soil degradation rate	6.2E-09	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.7E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.7E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-33. Chemical-Specific Inputs for Methyl ethyl ketone (78-93-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.1E-01	g/cm3	SCDM
HLC	Henry's law constant	5.6E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.8E-01	unitless	SCDM
MW	Molecular Weight	7.2E+01	g/mol	SCDM
Sol	Solubility	2.2E+05	mg/L	SCDM
VP	Vapor pressure	9.5E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-34. Chemical-Specific Inputs for 1,1,2-Trichloroethane (79-00-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.4E+00	g/cm3	SCDM
HLC	Henry's law constant	9.1E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	4.4E+03	mg/L	SCDM
VP	Vapor pressure	2.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	8.7E-13	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-35. Chemical-Specific Inputs for Trichloroethylene (79-01-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	1.0E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.7E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	1.1E+03	mg/L	SCDM
VP	Vapor pressure	7.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	8.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.9E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-36. Chemical-Specific Inputs for Acrylamide (79-06-1)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	1.0E-09	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-9.6E-01	unitless	SCDM
MW	Molecular Weight	7.1E+01	g/mol	SCDM
Sol	Solubility	6.4E+05	mg/L	SCDM
VP	Vapor pressure	7.0E-03	mmHg	SCDM
Density	Density of the chemical	1.1E+00	g/cm3	Merck
Kh	Hydrolysis rate	5.7E-10	sec-1	Kollig, 1993
K1	Aqueous degradation rate (low)	2.7E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	1.1E+01	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.
Ksg	Soil degradation rate	2.0E-06	sec-1	Calculated based on data in Howard, 1989

Table B-37. Chemical-Specific Inputs for Acrylic acid (79-10-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	1.2E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.5E-01	unitless	SCDM
MW	Molecular Weight	7.2E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	4.0E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	5.7E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	6.5E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-38. Chemical-Specific Inputs for 1,1,2,2-Tetrachloroethane (79-34-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	3.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.4E+00	unitless	SCDM
MW	Molecular Weight	1.7E+02	g/mol	SCDM
Sol	Solubility	3.0E+03	mg/L	SCDM
VP	Vapor pressure	4.6E+00	mmHg	SCDM
Kh	Hydrolysis rate	1.6E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.8E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.3E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-39. Chemical-Specific Inputs for 2-Nitropropane (79-46-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.8E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	8.7E-01	unitless	SCDM
MW	Molecular Weight	8.9E+01	g/mol	SCDM
Sol	Solubility	1.7E+04	mg/L	SCDM
VP	Vapor pressure	1.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-40. Chemical-Specific Inputs for Methyl methacrylate (80-62-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.4E-01	g/cm3	SCDM
HLC	Henry's law constant	3.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.4E+00	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	1.5E+04	mg/L	SCDM
VP	Vapor pressure	3.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.3E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-41. Chemical-Specific Inputs for Phthalic anhydride (85-44-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	1.6E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-6.2E-01	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	6.2E+03	mg/L	SCDM
VP	Vapor pressure	5.2E-04	mmHg	SCDM
Kh	Hydrolysis rate	1.6E-12	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.3E-04	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.8E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.7E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-42. Chemical-Specific Inputs for Hexachloro-1,3-butadiene (87-68-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	8.1E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.8E+00	unitless	SCDM
MW	Molecular Weight	2.6E+02	g/mol	SCDM
Sol	Solubility	3.2E+00	mg/L	SCDM
VP	Vapor pressure	2.2E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.0E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-43. Chemical-Specific Inputs for Naphthalene (91-20-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	4.8E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.4E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	3.1E+01	mg/L	SCDM
VP	Vapor pressure	8.5E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.7E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.3E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.4E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-44. Chemical-Specific Inputs for Benzidine (92-87-5)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.9E-11	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.7E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	5.0E+02	mg/L	SCDM
VP	Vapor pressure	8.0E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	1.3E+00	g/cm3	HSDB
Ksg	Soil degradation rate	1.0E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.6E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-45. Chemical-Specific Inputs for o-Dichlorobenzene (95-50-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	1.9E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.4E+00	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	1.6E+02	mg/L	SCDM
VP	Vapor pressure	1.4E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	5.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-46. Chemical-Specific Inputs for o-Toluidine (95-53-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	2.7E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.3E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	1.7E+04	mg/L	SCDM
VP	Vapor pressure	3.2E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	8.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-47. Chemical-Specific Inputs for 2-Chlorophenol (95-57-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	3.9E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	2.2E+04	mg/L	SCDM
VP	Vapor pressure	2.3E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.4E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	8.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-48. Chemical-Specific Inputs for 3,4-Dimethylphenol (95-65-8)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.8E-01	g/cm3	HSDB
MW	Molecular Weight	1.2E+02	g/mol	HSDB
Sol	Solubility	4.8E+03	mg/L	HSDB
VP	Vapor pressure	3.6E-02	mmHg	HSDB
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	2.2E+00	unitless	Hansch et al., 1995
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	5.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.
HLC	Henry's law constant	1.2E-06	atm-m3/mol	Calculated Based on Lyman, 1990.

Table B-49. Chemical-Specific Inputs for 1,2-Dibromo-3-chloropropane (96-12-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.1E+00	g/cm3	SCDM
HLC	Henry's law constant	1.5E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.3E+00	unitless	SCDM
MW	Molecular Weight	2.4E+02	g/mol	SCDM
Sol	Solubility	1.2E+03	mg/L	SCDM
VP	Vapor pressure	5.8E-01	mmHg	SCDM
Kh	Hydrolysis rate	1.3E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-50. Chemical-Specific Inputs for Furfural (98-01-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	4.0E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.1E-01	unitless	SCDM
MW	Molecular Weight	9.6E+01	g/mol	SCDM
Sol	Solubility	1.1E+05	mg/L	SCDM
VP	Vapor pressure	2.2E+00	mmHg	SCDM
Ksg	Soil degradation rate	1.0E-20	sec-1	no value for Ksg in existing hierarchy
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
K1	Aqueous degradation rate (low)	5.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-51. Chemical-Specific Inputs for Cumene (98-82-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.6E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E+00	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.6E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	6.1E+01	mg/L	SCDM
VP	Vapor pressure	4.5E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.0E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.9E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-52. Chemical-Specific Inputs for Nitrobenzene (98-95-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.4E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.8E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	2.1E+03	mg/L	SCDM
VP	Vapor pressure	2.5E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.1E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.3E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-53. Chemical-Specific Inputs for Ethylbenzene (100-41-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.7E-01	g/cm3	SCDM
HLC	Henry's law constant	7.9E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.1E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	1.7E+02	mg/L	SCDM
VP	Vapor pressure	9.6E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	8.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.1E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.8E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-54. Chemical-Specific Inputs for Styrene (100-42-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.1E-01	g/cm3	SCDM
HLC	Henry's law constant	2.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.9E+00	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	3.1E+02	mg/L	SCDM
VP	Vapor pressure	6.1E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.1E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-55. Chemical-Specific Inputs for p-Dichlorobenzene (106-46-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.4E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.4E+00	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	7.4E+01	mg/L	SCDM
VP	Vapor pressure	1.0E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.3E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.4E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.7E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-56. Chemical-Specific Inputs for 1,2-Epoxybutane (106-88-7)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	8.4E-01	g/cm3	HSDB
VP	Vapor pressure	1.8E+02	mmHg	HSDB
Ksg	Soil degradation rate	6.2E-07	sec-1	Howard et al, 1991
HLC	Henry's law constant	1.8E-04	atm-m3/mol	Chemfate
LogKow	Octanol-water partition coeficient	2.6E-01	unitless	Chemfate
MW	Molecular Weight	7.2E+01	g/mol	Chemfate
Sol	Solubility	9.5E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	4.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-57. Chemical-Specific Inputs for Epichlorohydrin (106-89-8)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.0E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E-01	unitless	SCDM
MW	Molecular Weight	9.3E+01	g/mol	SCDM
Sol	Solubility	6.6E+04	mg/L	SCDM
VP	Vapor pressure	1.6E+01	mmHg	SCDM
Density	Density of the chemical	1.2E+00	g/cm3	Merck
Kh	Hydrolysis rate	9.8E-07	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-58. Chemical-Specific Inputs for Ethylene dibromide (106-93-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.2E+00	g/cm3	SCDM
HLC	Henry's law constant	7.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.9E+02	g/mol	SCDM
Sol	Solubility	4.2E+03	mg/L	SCDM
VP	Vapor pressure	1.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	2.0E-08	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	5.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-59. Chemical-Specific Inputs for 1,3-Butadiene (106-99-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	6.1E-01	g/cm3	SCDM
HLC	Henry's law constant	7.4E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	5.4E+01	g/mol	SCDM
Sol	Solubility	7.4E+02	mg/L	SCDM
VP	Vapor pressure	2.1E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-60. Chemical-Specific Inputs for Acrolein (107-02-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.4E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.0E-02	unitless	SCDM
MW	Molecular Weight	5.6E+01	g/mol	SCDM
Sol	Solubility	2.1E+05	mg/L	SCDM
VP	Vapor pressure	2.7E+02	mmHg	SCDM
Kh	Hydrolysis rate	2.1E+01	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	7.8E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-61. Chemical-Specific Inputs for Allyl chloride (107-05-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.4E-01	g/cm3	SCDM
HLC	Henry's law constant	1.1E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	7.7E+01	g/mol	SCDM
Sol	Solubility	3.4E+03	mg/L	SCDM
VP	Vapor pressure	3.7E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.8E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-62. Chemical-Specific Inputs for 1,2-Dichloroethane (107-06-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	9.8E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	9.9E+01	g/mol	SCDM
Sol	Solubility	8.5E+03	mg/L	SCDM
VP	Vapor pressure	7.9E+01	mmHg	SCDM
Kh	Hydrolysis rate	3.0E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	9.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-63. Chemical-Specific Inputs for Acrylonitrile (107-13-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.1E-01	g/cm3	SCDM
HLC	Henry's law constant	1.0E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E-01	unitless	SCDM
MW	Molecular Weight	5.3E+01	g/mol	SCDM
Sol	Solubility	7.4E+04	mg/L	SCDM
VP	Vapor pressure	1.1E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.5E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-64. Chemical-Specific Inputs for Ethylene glycol (107-21-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	6.0E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.4E+00	unitless	SCDM
MW	Molecular Weight	6.2E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.2E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	6.7E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.2E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.4E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-65. Chemical-Specific Inputs for Vinyl acetate (108-05-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.3E-01	g/cm3	SCDM
HLC	Henry's law constant	5.1E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	7.3E-01	unitless	SCDM
MW	Molecular Weight	8.6E+01	g/mol	SCDM
Sol	Solubility	2.0E+04	mg/L	SCDM
VP	Vapor pressure	9.0E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-66. Chemical-Specific Inputs for Methyl isobutyl ketone (108-10-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.0E-01	g/cm3	SCDM
HLC	Henry's law constant	1.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.2E+00	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	1.9E+04	mg/L	SCDM
VP	Vapor pressure	2.0E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	7.4E-01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.7E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-67. Chemical-Specific Inputs for Toluene (108-88-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.7E-01	g/cm3	SCDM
HLC	Henry's law constant	6.6E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.8E+00	unitless	SCDM
MW	Molecular Weight	9.2E+01	g/mol	SCDM
Sol	Solubility	5.3E+02	mg/L	SCDM
VP	Vapor pressure	2.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.6E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.4E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-68. Chemical-Specific Inputs for Chlorobenzene (108-90-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	3.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.9E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	4.7E+02	mg/L	SCDM
VP	Vapor pressure	1.2E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.4E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.9E-01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-69. Chemical-Specific Inputs for Cyclohexanol (108-93-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.6E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
VP	Vapor pressure	8.0E-01	mmHg	HSDB
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	1.2E+00	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.0E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	1.0E+02	g/mol	Chemfate
Sol	Solubility	4.3E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	5.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.1E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-70. Chemical-Specific Inputs for Phenol (108-95-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	4.0E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	9.4E+01	g/mol	SCDM
Sol	Solubility	8.3E+04	mg/L	SCDM
VP	Vapor pressure	2.8E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	8.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.3E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-71. Chemical-Specific Inputs for 2-Methoxyethanol (109-86-4)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.6E-01	g/cm3	HSDB
Sol	Solubility	1.0E+06	mg/L	HSDB
VP	Vapor pressure	6.2E+00	mmHg	HSDB
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	-7.7E-01	unitless	Hansch et al., 1995
HLC	Henry's law constant	8.1E-08	atm-m3/mol	Chemfate
MW	Molecular Weight	7.6E+01	g/mol	Chemfate
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-72. Chemical-Specific Inputs for 2-Methoxyethanol acetate (110-49-6)

Parameter	Definition	Value	Units	Reference
LogKow	Octanol-water partition coeficient	1.0E-01	unitless	KowWIN
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	1.0E+00	g/cm3	HSDB
MW	Molecular Weight	1.2E+02	g/mol	HSDB
Sol	Solubility	1.0E+06	mg/L	HSDB
VP	Vapor pressure	2.0E+00	mmHg	HSDB
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.7E-06	cm2/s	Calculated based on WATER9, 2001.
HLC	Henry's law constant	3.1E-07	atm-m3/mol	Calculated Based on Lyman, 1990.

Table B-73. Chemical-Specific Inputs for n-Hexane (110-54-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	6.5E-01	g/cm3	SCDM
HLC	Henry's law constant	1.4E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.0E+00	unitless	SCDM
MW	Molecular Weight	8.6E+01	g/mol	SCDM
Sol	Solubility	1.2E+01	mg/L	SCDM
VP	Vapor pressure	1.5E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.5E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-74. Chemical-Specific Inputs for 2-Ethoxyethanol (110-80-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.3E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.0E-01	unitless	SCDM
MW	Molecular Weight	9.0E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	5.3E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-75. Chemical-Specific Inputs for Pyridine (110-86-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.8E-01	g/cm3	SCDM
HLC	Henry's law constant	8.9E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.7E-01	unitless	SCDM
MW	Molecular Weight	7.9E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	2.1E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-76. Chemical-Specific Inputs for 2-Ethoxyethanol acetate (111-15-9)

Parameter	Definition	Value	Units	Reference
LogKow	Octanol-water partition coeficient	5.9E-01	unitless	KowWIN
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.7E-01	g/cm3	HSDB
HLC	Henry's law constant	1.8E-06	atm-m3/mol	HSDB
Sol	Solubility	2.3E+05	mg/L	HSDB
VP	Vapor pressure	2.3E+00	mmHg	HSDB
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
MW	Molecular Weight	1.3E+02	g/mol	Chemfate
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.0E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-77. Chemical-Specific Inputs for Hexachlorobenzene (118-74-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.0E+00	g/cm3	SCDM
HLC	Henry's law constant	1.3E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	5.9E+00	unitless	SCDM
MW	Molecular Weight	2.8E+02	g/mol	SCDM
Sol	Solubility	5.0E-03	mg/L	SCDM
VP	Vapor pressure	1.8E-05	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.8E-09	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	9.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-78. Chemical-Specific Inputs for 1,2,4-Trichlorobenzene (120-82-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	1.4E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.0E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	3.5E+01	mg/L	SCDM
VP	Vapor pressure	4.3E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.7E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-79. Chemical-Specific Inputs for 2,4-Dinitrotoluene (121-14-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	9.3E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	2.7E+02	mg/L	SCDM
VP	Vapor pressure	1.5E-04	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-80. Chemical-Specific Inputs for Triethylamine (121-44-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.3E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	0.0E+00	sec-1	HSDB
VP	Vapor pressure	5.7E+01	mmHg	HSDB
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.4E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	1.0E+02	g/mol	Chemfate
Sol	Solubility	5.5E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	1.1E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-81. Chemical-Specific Inputs for 1,2-Diphenylhydrazine (122-66-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	1.5E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.9E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	6.8E+01	mg/L	SCDM
VP	Vapor pressure	4.3E-04	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.9E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.9E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	1.4E+01	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	5.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.3E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-82. Chemical-Specific Inputs for 1,4-Dioxane (123-91-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	4.8E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-3.9E-01	unitless	SCDM
MW	Molecular Weight	8.8E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	3.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-83. Chemical-Specific Inputs for Chlorodibromomethane (124-48-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.5E+00	g/cm3	SCDM
HLC	Henry's law constant	7.8E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.2E+00	unitless	SCDM
MW	Molecular Weight	2.1E+02	g/mol	SCDM
Sol	Solubility	2.6E+03	mg/L	SCDM
VP	Vapor pressure	4.9E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.5E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-84. Chemical-Specific Inputs for Chloroprene (126-99-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.6E-01	g/cm3	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	8.9E+01	g/mol	SCDM
Sol	Solubility	1.7E+03	mg/L	SCDM
VP	Vapor pressure	2.1E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
HLC	Henry's law constant	1.2E-02	atm-m3/mol	Chemfate
K1	Aqueous degradation rate (low)	2.2E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	7.8E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-85. Chemical-Specific Inputs for Tetrachloroethylene (127-18-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	1.8E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.7E+00	unitless	SCDM
MW	Molecular Weight	1.7E+02	g/mol	SCDM
Sol	Solubility	2.0E+02	mg/L	SCDM
VP	Vapor pressure	1.9E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.1E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-86. Chemical-Specific Inputs for 1,1,1,2-Tetrachloroethane (630-20-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	2.4E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.6E+00	unitless	SCDM
MW	Molecular Weight	1.7E+02	g/mol	SCDM
Sol	Solubility	1.1E+03	mg/L	SCDM
VP	Vapor pressure	1.2E+01	mmHg	SCDM
Kh	Hydrolysis rate	4.3E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.2E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-87. Chemical-Specific Inputs for N-Nitrosodi-n-butylamine (924-16-3)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.2E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.4E+00	unitless	SCDM
MW	Molecular Weight	1.6E+02	g/mol	SCDM
Sol	Solubility	1.3E+03	mg/L	SCDM
VP	Vapor pressure	3.0E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.0E-01	g/cm3	HSDB
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-04	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	6.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-88. Chemical-Specific Inputs for N-Nitrosopyrrolidine (930-55-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	1.2E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.9E-01	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.2E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-04	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-89. Chemical-Specific Inputs for Cresols (total) (1319-77-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	9.5E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.3E+04	mg/L	SCDM
VP	Vapor pressure	1.8E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.8E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.7E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.3E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-90. Chemical-Specific Inputs for Xylenes (1330-20-7)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	6.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.2E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	1.8E+02	mg/L	SCDM
VP	Vapor pressure	8.0E+00	mmHg	SCDM
Density	Density of the chemical	8.7E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.8E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-91. Chemical-Specific Inputs for Methyl tert-butyl ether (1634-04-4)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	7.4E-01	g/cm3	HSDB
VP	Vapor pressure	2.5E+02	mmHg	HSDB
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	9.4E-01	unitless	Hansch et al., 1995
HLC	Henry's law constant	5.9E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	8.8E+01	g/mol	Chemfate
Sol	Solubility	5.1E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	7.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-92. Chemical-Specific Inputs for 2,3,7,8-TCDD (1746-01-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.8E+00	g/cm3	Mackay et al, 1992
Ksg	Soil degradation rate	1.4E-08	sec-1	Howard et al, 1991
HLC	Henry's law constant	3.3E-05	atm-m3/mol	Dioxin Reassessment
Kh	Hydrolysis rate	0.0E+00	sec-1	Dioxin Reassessment
LogKow	Octanol-water partition coeficient	6.8E+00	unitless	Dioxin Reassessment
MW	Molecular Weight	3.2E+02	g/mol	Dioxin Reassessment
Sol	Solubility	1.9E-05	mg/L	Dioxin Reassessment
VP	Vapor pressure	1.5E-09	mmHg	Dioxin Reassessment
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Dw	Diffusion coefficient in water	6.8E-06	cm2/s	Calculated based on WATER9, 2001.
Da	Diffusivity of chemical in air	4.7E-02	cm2/s	Calculated based on EPA's Dioxin Reassessment, 2000.

Table B-93. Chemical-Specific Inputs for Mercury (7439-97-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.4E+01	g/cm3	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	not applicable for metallic species
Ksg	Soil degradation rate	0.0E+00	sec-1	not applicable for metallic species
HLC	Henry's law constant	7.1E-03	atm-m3/mol	MRTC
LogKd	soil-water partition coeficient	3.0E+00	unitless	MRTC
MW	Molecular Weight	2.0E+02	g/mol	MRTC
Sol	Solubility	5.6E-02	mg/L	Merck
VP	Vapor pressure	2.0E-03	mmHg	Merck
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-04	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Dw	Diffusion coefficient in water	3.0E-05	cm2/s	Calculated based on WATER9, 2001.
Da	Diffusivity of chemical in air	5.5E-02	cm2/s	Calculated based on EPA, 1987.

Table B-94. Chemical-Specific Inputs for Divalent mercury (7439-97-7)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	not applicable for metallic species
Ksg	Soil degradation rate	0.0E+00	sec-1	not applicable for metallic species
HLC	Henry's law constant	7.1E-10	atm-m3/mol	MRTC
LogKd	soil-water partition coeficient	4.8E+00	unitless	MRTC
MW	Molecular Weight	2.0E+02	g/mol	MRTC
Sol	Solubility	7.4E+04	mg/L	Merck
Density	Density of the chemical	5.6E+00	g/cm3	HSDB
VP	Vapor pressure	1.0E+00	mmHg	HSDB
Dw	Diffusion coefficient in water	1.8E-05	cm2/s	Calculated based on WATER9, 2001.
Da	Diffusivity of chemical in air	5.5E-02	cm2/s	Calculated based on EPA, 1987.
K1	Aqueous degradation rate (low)			
Kmax	Aqueous degradation rate (max)			
VP Coeff A	Antoine's coefficient A			
VP Coeff B	Antoine's coefficient B			
VP Coeff C	Antoine's coefficient C			

Table B-95. Chemical-Specific Inputs for cis-1,3-Dichloropropylene (10061-01-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.7E+03	mg/L	SCDM
VP	Vapor pressure	3.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	1.3E-06	sec-1	Kollig, 1993
HLC	Henry's law constant	2.4E-03	atm-m3/mol	HSDB
Ksg	Soil degradation rate	7.1E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-96. Chemical-Specific Inputs for trans-1,3-Dichloropropylene (10061-02-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.7E+03	mg/L	SCDM
VP	Vapor pressure	2.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	1.3E-06	sec-1	Kollig, 1993
HLC	Henry's law constant	1.8E-03	atm-m3/mol	HSDB
Ksg	Soil degradation rate	7.1E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

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