Appendix A: Substance-independent input data

Parameter	Unit	Value
ENVIRONMENTAL DISTRIBUTION		
Density of the solid phase	$kg \cdot m^{-3}$	2500
Density of water	$kg \cdot m^{-3}$	1000
Density of air	$kg \cdot m^{-3}$	1.3
Temperature at the continental air-water interface	K	285
Temperature at the moderate air-water interface	K	285
Temperature at the arctic air-water interface	K	263
Temperature at the tropic air-water interface	K	298
Constant of Junge equation	$Pa \cdot m$	[a]
Surface area of aerosol particles	$m^2.m^{-3}$	[a]
Gas constant	$Pa.m^3.mol^{-1}.K^{-1}$	8.314
Volume fraction of solids in suspended matter	$m_{solid}^3 . m_{susp}^{-3}$	0.1
Volume fraction of water in suspended matter	$m_{water}^3 . m_{susp}^{-3}$	0.9
Weight fraction of organic carbon in suspended solids	$kg_{oc} . kg_{solid}^{-1}$	0.1
Volume fraction of solids in sediment	$m_{solid}^3 . m_{sed}^{-3}$	0.2
Volume fraction of water in sediment	$m_{water}^3 . m_{sed}^{-3}$	0.8
Weight fraction of organic carbon in sediment solids	$kg_{oc} . kg_{solid}^{-1}$	0.05
Volume fraction of solids in soil	$m_{solid}^3 . m_{soil}^{-3}$	0.6
Volume fraction of water in soil	$m_{water}^3 . m_{soil}^{-3}$	0.2
Volume fraction of air in soil	$m_{water}^3 . m_{soil}^{-3}$	0.2
Weight fraction of organic carbon in sediment solids	$kg_{oc} . kg_{solid}^{-1}$	0.02
Concentration of OH-radicals in atmosphere	$molecules.m^{-3}$	$5 \cdot 10^{11}$
Fraction of sediment compartment that is aerated	$m^3.m^{-3}$	0.1
Atmospheric mixing height at all scales	m	1000
Wind speed at all scales	$m.d^{-1}$	$2.59 \cdot 10^5$
Aerosol-deposition velocity at all scales	$m.d^{-1}$	86.4
Aerosol-collection efficiency at all scales	-	$2 \cdot 10^5$
Average daily precipitation at continental scale and moderate zone	$mm \cdot yr^{-1}$	700
Average daily precipitation in arctic zone	$mm \cdot yr^{-1}$	250
Average daily precipitation in tropic zone	$mm \cdot yr^{-1}$	1300
Concentration of biota in water at all scales	$kg_{wwt} \cdot m^{-3}$	0.1
Total area of the continental scale	km^2	$7.16 \cdot 10^6$
Total area of the moderate scale[b]	km^2	$4.25 \cdot 10^7$
Total area of the arctic scale	km^2	$7.78 \cdot 10^7$
Total area of the tropic scale	km^2	$1.28 \cdot 10^8$
Fraction of the continent that is fresh water	-	0.015
Fraction of the continent that is seawater	-	0.5
Fraction of the continent that is natural soil	-	0.3
Fraction of the continent that is agricultural soil	-	0.135
Fraction of the continent that is industrial soil	-	0.05
Fraction of the moderate zone that is water	-	0.5
Fraction of the moderate zone that is soil	-	0.5
Fraction of the arctic zone that is water	-	0.6
Fraction of the arctic zone that is soil	-	0.4
Fraction of the tropic zone that is water	-	0.7
Fraction of the tropic zone that is soil	-	0.3
Water depth of fresh water at continental scale	m	3
Water depth of sea water at continental scale	m	200
Water depth of sea water at global zones	m	1000
Suspended solids conc. continental fresh water	$kg_{dwt}.m^{-3}$	0.025
Suspended solids conc. in sea water at all scales	$kg_{dwt}.m^{-3}$	0.005
Sediment mixing depth at all scales	m	0.03
Settling velocity of suspended particles at all scales	$m.d^{-1}$	2.5
Production rate of susp. matter in continental fresh water	$kg_{dwt}.m^{-2}.yr^{-1}$	0.01
Production rate of susp. matter in seawater at all scales	$kg_{dwt}.m^{-2}.yr^{-1}$	0.001
Fraction of rain water that infiltrates the soil at all scales	-	0.25
Fraction of wet prec. that runs off soil to water at all scales	-	0.25
Soil-erosion rate at all scales	$m.d^{-1}$	$8.2 \cdot 10^{-8}$
Enthalphy of vaporation	$kJ.mol^{-1}$	50
Enthalphy of solution	$kJ.mol^{-1}$	10
Air-film partial mass-transfer coefficient at all scales (air-water and air-soil interfaces)	$m.d^{-1}$	120
Water-film partial mass-transfer coefficient at all scales (air-water interface)	$m.d^{-1}$	1.2
Soil-air partial mass-transfer coefficient at all scales (air-soil interface)	$m.d^{-1}$	0.48
Soil water-water film partial-mass transfer coefficient (air-soil interface)	$m.d^{-1}$	$4.8 \cdot 10^{-5}$

Water-film partial mass-transfer coefficient at all scales (sediment-water interface)	$m.d^{-1}$	0.24
Pore water partial mass-transfer coefficient (sediment-water interface)	$m.d^{-1}$	$2.4 \cdot 10^{-3}$

[a] By default, the product of CONjunge and SURFaer is set to $1 \cdot 10^{-4}$ Pa, although CONjunge is (partly) substance-dependent; [b] the area of the continental scale is not included in the area of the moderate scale.

Parameter	Unit	Value
HUMAN EXPOSURE ASSESSMENT		
Volume fraction of fat in plant roots	$m^3.m^{-3}$	0.005
Volume fraction of water in plant roots	$m^3.m^{-3}$	0.93
Bulk densitiy of plant root tissue	$kg_{wwt}.m^{-3}$	1000
Volume fraction of fat in plant leafs	$m^3.m^{-3}$	0.01
Volume fraction of water in plant leafs	$m^3.m^{-3}$	0.65
Volume fraction of air in plant leafs	$m^3.m^{-3}$	0.3
Bulk densitiy of plant leaf tissue	$kg_{wwt}.m^{-3}$	800
Leaf surface area	m^2	5
Shoot volume	m^3	0.002
Transpiration stream	$m^3 \cdot d^{-1}$	0.001
Correction factor for differences between plant lipids and octanol	-	0.95
Growth-rate constant for dilution by growth	d^{-1}	0.035
Daily intake of grass by cattle	$kg_{dwt} \cdot d^{-1}$	72.5
Daily intake of soil by cattle	$kg_{dwt} \cdot d^{-1}$	0.4
Daily intake of air by cattle	$m^3 \cdot d^{-1}$	122
Daily intake of drinking water by cattle	$m^3 \cdot d^{-1}$	0.055
Conversion dry weight to wet weight grass	$kg_{wwt}.kg_{dwt}^{-1}$	4
Fraction drinking water from groundwater	-	0.57
Fraction drinking water from surface water	-	0.43
Daily intake of drinking water	$l.d^{-1}$	1.14
Daily intake of fish[a]	$kg_{wwt}.d^{-1}$	0.03
Daily intake of leaf crops (incl. fruit and cereals)[b]	$kg_{wwt}.d^{-1}$	0.77
Daily intake of root crops[b]	$kg_{wwt}.d^{-1}$	0.18
Daily intake of meat	$kg_{wwt}.d^{-1}$	0.26
Daily intake of dairy products	$kg_{wwt}.d^{-1}$	0.28
Daily inhalation rate	$m^3.d^{-1}$	12.7
Body weight	kg	70
Daily soil ingestion[c]	$mg_{wwt}.d^{-1}$	50

[a] it is assumed that 90% of the total fish intake (kg_{wwt}) on the continental scale are salt water species and 10% fresh water species; [b] an edible fraction of 0.8 for fruit, vegetables and root crops is assumed; [c] it is assumed that on the continental scale all ingested soil comes from industrial/urban soils.

Appendix B: Substance-specific input data

Table B.1a: Substance-specific input parameters for metals

Compound name	Unit	Antimony	Arsenic	Barium	Beryllium	Cadmium	Chromium III	ChromiumVI	Cobalt	Copper	Source
CAS nr.	-	7440-36-0	7440-38-2	7440-39-3	7440-41-7	7440-43-9	7440-47-3	7440-47-3	7440-48-4	7440-50-8	
Effects assessment											1-9
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$8.6 \cdot 10^{-10}$	$2.14 \cdot 10^{-9}$	$7.0 \cdot 10^{-8}$	$5.0 \cdot 10^{-10}$	$1.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-9}$	$1.4 \cdot 10^{-9}$	$1.4 \cdot 10^{-7}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$3.2 \cdot 10^{-9}$	$2.5 \cdot 10^{-13}$	$5.0 \cdot 10^{-10}$	$4.0 \cdot 10^{-13}$	$6.0 \cdot 10^{-13}$		$2.5 \cdot 10^{-14}$	$5.0 \cdot 10^{-12}$	$2.0 \cdot 10^{-11}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$4.6 \cdot 10^{-4}$	$2.4 \cdot 10^{-5}$	$5.8 \cdot 10^{-5}$	$1.6 \cdot 10^{-7}$	$3.4 \cdot 10^{-7}$	$3.4 \cdot 10^{-5}$	$8.5 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$	$1.1 \cdot 10^{-6}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	$3.6 \cdot 10^{-7}$	EP[a]	EP[a]	$4.6 \cdot 10^{-7}$	$3.3 \cdot 10^{-7}$	$3.3 \cdot 10^{-7}$	EP[a]	$7.7 \cdot 10^{-6}$	
Physico-chemical properties											10
molecular weight	$g.mol^{-1}$	121.76	74.92	137.33	9.01	112.41	52	52	5893	63.55	
melting point	°C	630.74	817	725	1278	320.9	1900	1900	1495	1083	
Partition coefficients											11, 12
solid-water partition coefficient soil	$l.kg^{-1}$	85	3337	60	38	152	8427	8427	40	221	
solid-water partition coefficient sediment	$l.kg^{-1}$	2570	6607	1000	603	85114	190546	190546	3981	33884	
solid-water partition coefficient suspended matter	$l.kg^{-1}$	3715	10000	1349	851	128825	288403	288403	3890	50119	
aerosol collection efficiency		$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	
fraction of aerosol bounded substance	-	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95	
Exposure assessment											13-23
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	80	150	216	19	38	40	40	1	120	
bioconcentration factor from soil to plant roots	$kg(wwt).kg(wwt)^{-1}$	$2.0 \cdot 10^{-2}$	$1.6 \cdot 10^{-2}$	$2.0 \cdot 10^{-2}$	$6.1 \cdot 10^{-3}$	$1.4 \cdot 10^{-1}$	$4.0 \cdot 10^{-3}$	$4.0 \cdot 10^{-3}$	$6.1 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	
bioconcentration factor from soil to plant leafs	$kg(wwt).kg(wwt)^{-1}$	$1.2 \cdot 10^{-2}$	$9.4 \cdot 10^{-3}$	$5.9 \cdot 10^{-4}$	$3.5 \cdot 10^{-3}$	$1.8 \cdot 10^{-2}$	$2.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	$1.8 \cdot 10^{-3}$	$1.2 \cdot 10^{-2}$	
biotransfer factor for meat	$d.kg(food)^{-1}$	$3.9 \cdot 10^{-4}$	$2.2 \cdot 10^{-4}$	$9.7 \cdot 10^{-5}$	$3.2 \cdot 10^{-6}$	$5.3 \cdot 10^{-3}$	$9.2 \cdot 10^{-3}$	$9.2 \cdot 10^{-3}$	$9.7 \cdot 10^{-3}$	$1.3 \cdot 10^{-2}$	
biotransfer factor for milk	$d.kg(food)^{-1}$	$1.1 \cdot 10^{-4}$	$6.0 \cdot 10^{-5}$	$3.4 \cdot 10^{-4}$	$8.8 \cdot 10^{-7}$	$1.5 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$2.8 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$	
bioavailability for human inhalation	-		0.4	0.75	0.5	0.15	0.1	0.25			
bioavailability for human oral uptake	-	0.1	0.9	0.1	0.001	0.05	0.01	0.05		0.4	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] RIZA (1999); [2] Vermeire et al. (1991); [3] Huijbregts (1999); [4] USEPA (1998b); [5] WHO (1987a); [6] JECFA (1989); [7] Environmental Defense Fund (1999); [8] Janssen et al. (1995); [9] Janus et al. (1994); [10] Cambridgesoft Corporation (1998); [11] Crommentuijn et al. (1997a); [12] De Groot et al. (1998); [13] Slooff et al. (1992c); [14] Owen (1990); [15] Spectrum Research (1992); [16] Van de Plassche (1994); [17] Slooff et al. (1990b); [18] Van de Berg (1995); [19] Ng (1982); [20] Slooff et al. (1992b); [21] Owen (1990); [22] Slooff et al. (1990a); [23] personal assessment

Table B.1b: Substance-specific input parameters for metals

Compound name	Unit	Lead	Mercury	Methyl-mercury	Molyb-denum	Nickel	Selenium	Thallium	Tin	Vanadium	Zinc	Source
CAS nr.	-	7439-92-1	7439-97-6	22967-92-6	7439-98-7	7440-02-0	7782-49-2	7440-28-0	7440-31-5	7440-62-2	7440-66-6	
Effects assessment												1-11
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.6 \cdot 10^{-9}$	$7.2 \cdot 10^{-10}$	$4.71 \cdot 10^{-10}$	$1.0 \cdot 10^{-8}$	$5.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-9}$	$2.0 \cdot 10^{-10}$	$2.0 \cdot 10^{-6}$	$2.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-6}$	
Inhalatory Human Limit Value	$kg.m^{-3}$		$3.0 \cdot 10^{-10}$	$1.0 \cdot 10^{-9}$			$2.5 \cdot 10^{-12}$	$8.0 \cdot 10^{-11}$		$1.0 \cdot 10^{-9}$	$9.0 \cdot 10^{-10}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$1.1 \cdot 10^{-5}$	$1.3 \cdot 10^{-7}$	$1.0 \cdot 10^{-8}$	$2.9 \cdot 10^{-5}$	$1.8 \cdot 10^{-6}$	$5.3 \cdot 10^{-6}$	$1.6 \cdot 10^{-6}$	$1.8 \cdot 10^{-5}$	$8.2 \cdot 10^{-7}$	$6.6 \cdot 10^{-6}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$4.4 \cdot 10^{-5}$	$1.5 \cdot 10^{-9}$	EP[a]	EP[a]	$7.4 \cdot 10^{-7}$	EP[a]	EP[a]	EP[a]	EP[a]	$6.7 \cdot 10^{-6}$	
Physico-chemical properties												12, 13
molecular weight	$g.mol^{-1}$	207.2	200.59	215.62	95.94	58.69	78.96	204.38	118.69	50.94	65.39	
melting point	°C	327.43	-38.9	-38.9	2622	1455	217	302	231.9	1344	419.5	
Partition coefficients												14, 15
solid-water partition coefficient soil	$l.kg^{-1}$	4332	170	170	871	359	20	334	4332	309	334	
solid-water partition coefficient sediment	$l.kg^{-1}$	$4.3 \cdot 10^{5}$	$1.1 \cdot 10^{5}$	112201.8	851	$5.2 \cdot 10^{3}$	417	$1.0 \cdot 10^{3}$	$1.2 \cdot 10^{6}$	$3.9 \cdot 10^{3}$	$7.2 \cdot 10^{4}$	
solid-water partition coefficient suspended matter	$l.kg^{-1}$	$6.5 \cdot 10^{5}$	$1.7 \cdot 10^{5}$	169824.4	$1.1 \cdot 10^{3}$	$7.9 \cdot 10^{3}$	589	$1.5 \cdot 10^{3}$	$3.7 \cdot 10^{5}$	$5.5 \cdot 10^{3}$	$1.1 \cdot 10^{5}$	
aerosol collection efficiency	-	$1.0 \cdot 10^{5}$	$2.0 \cdot 10^{5}$	$2.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	$1.0 \cdot 10^{5}$	
fraction of aerosol bounded substance	-	0.95	0.05	0.05	0.95	0.95	0.95	0.95	0.95	0.95	0.95	
Exposure assessment												5, 16-29
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	500	3030	21700	216	87	500	250	216	200	1000	
bioconcentration factor from soil to plant roots	$kg(wwt).kg(wwt)^{-1}$	$6.1 \cdot 10^{-3}$	$6.1 \cdot 10^{-3}$	$6.1 \cdot 10^{-3}$	$6.1 \cdot 10^{-2}$	$2.0 \cdot 10^{-2}$	$2.0 \cdot 10^{-2}$	$6.1 \cdot 10^{-3}$	$6.1 \cdot 10^{-3}$	$6.1 \cdot 10^{-2}$	$8.1 \cdot 10^{-2}$	
bioconcentration factor from soil to plant leafs	$kg(wwt).kg(wwt)^{-1}$	$1.2 \cdot 10^{-4}$	$1.8 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	$8.2 \cdot 10^{-3}$	$1.2 \cdot 10^{-2}$	$3.5 \cdot 10^{-1}$	$1.8 \cdot 10^{-3}$	$3.5 \cdot 10^{-1}$	$1.2 \cdot 10^{-2}$	
biotransfer factor for meat	$d.kg(food)^{-1}$	$1.0 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$	$1.2 \cdot 10^{-2}$	$6.8 \cdot 10^{-3}$	$2.0 \cdot 10^{-3}$	$1.4 \cdot 10^{-2}$	$6.7 \cdot 10^{-3}$	$4.2 \cdot 10^{-3}$	$6.7 \cdot 10^{-4}$	$1.2 \cdot 10^{-1}$	
biotransfer factor for milk	$d.kg(food)^{-1}$	$2.5 \cdot 10^{-4}$	$4.6 \cdot 10^{-4}$	$3.3 \cdot 10^{-3}$	$1.4 \cdot 10^{-3}$	$9.7 \cdot 10^{-4}$	$3.9 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$	$9.7 \cdot 10^{-3}$	
respirable fraction of inhaled substance	-							0.35				
bioavailability for human inhalation	-	0.5	0.75	1.0		0.06	0.3	1		0.25	0.5	
bioavailability for human oral uptake	-	0.1	0.0001	0.95		0.05	0.6		0.05	0.02	0.5	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] RIZA (1999); [2] USEPA (1998b); [3] WHO (1987a); [4] Vermeire et al. (1991); [5] Janssen et al. (1998); [6] JECFA (1982); [7] JECFA (1986); [8] JECFA (1989); [9] Environmental Defense Fund (1999); [10] Huijbregts (1999); [11] Janus et al. (1994); [12] Cambridgesoft Corporation (1998); [13] Lide (1993); [14] Crommentuijn et al. (1997a); [15] De Groot et al. (1998); [16] Guinée et al. (1996a); [17] Bockting et al. (1996); [18] Slooff et al. (1995); [19] Van de Plassche et al. (1992); [20] Slooff et al. (1992a); [21] Slooff et al. (1993); [22] Owen (1990); [23] Van de Berg (1995); [24] Ng (1982); [25] WHO (1995a); [26] WHO (1996a); [27] Slooff et al. (1993); [28] Spectrum Research (1992); [29] personal assessment

Table B.2: Substance-specific input parameters for inorganics

Compound name	Unit	ammonia (anhydrous)	nitrogen dioxide	sulphur dioxide	hydrogen sulphide	hydrogen chloride	primary fine particulate matter (PM10)	Source
CAS nr.	-	7664-41-7	10102-44-0	7446-09-5	7783-06-4	7647-01-0		
Effects assessment								1-3
Inhalatory Human Limit Value	$kg.m^{-3}$	$1 \cdot 10^{-7}$	$4 \cdot 10^{-8}$	$3.5 \cdot 10^{-7}$	$1.5 \cdot 10^{-7}$	$2 \cdot 10^{-8}$	$4 \cdot 10^{-8}$	
Physico-chemical properties								2, 5-9
molecular weight	$g.mol^{-1}$	17.03	46.02	64.06	34.08	36.461		
melting point	°C	-77.7	-11.2	-75.51	-85.6	-114.24		
vapor pressure (25 °C)	Pa	$9.2 \cdot 10^{5}$	$1.4 \cdot 10^{5}$	$3.1 \cdot 10^{5}$	$2.0 \cdot 10^{6}$	$1.4 \cdot 10^{5}$	$1 \cdot 10^{-30}$	
solubility (25 °C)	$mg.l^{-1}$	$5.7 \cdot 10^{5}$	$1.0 \cdot 10^{6}$	$1.1 \cdot 10^{5}$	$2.9 \cdot 10^{3}$	$6.2 \cdot 10^{5}$	$1 \cdot 10^{-13}$	
Partition coefficients								7, 10-12
Henry's law constant (25 °C)	$Pa.m^3.mol^{-1}$				$5.5 \cdot 10^{7}$			
aerosol deposition velocity	$m.s^{-1}$						$1.5 \cdot 10^{-3}$	
scavenging ratio	-	$1.4 \cdot 10^{6}$		$3 \cdot 10^{5}$	[a] $3 \cdot 10^{5}$	[a] $1.4 \cdot 10^{6}$	$3.5 \cdot 10^{5}$	
fraction of aerosol bounded substance	-						1	
Degradation rates								12-14
reaction half-life in air	d	$1 \cdot 10^{30}$		3.6			$1 \cdot 10^{30}$	
hydroxyl radical reaction in air	$cm^3.molec^{-1}.sec^{-1}$		$1.1 \cdot 10^{-11}$		$4.8 \cdot 10^{-12}$	$8.1 \cdot 10^{-13}$		

[a] It is assumed that HCl has a scavenging ratio equal to HNO_3 and H_2S has a scavenging ratio equal to SO_2 (values for HNO_3 and SO_2 taken from Barrett & Berge, 1996); [1] WHO-EURO (1987); [2] WHO (1997a); [3] USEPA (1998b); [4] Guinée et al. (1996a); [5] Verschueren (1996); [6] Cambridgesoft Corporation (1998); [7] Slooff et al. (1991a); [8] University of Akron (1998); [9] Howard Hughes Medical Institute (1998); [10] D. van de Meent (pers. comm.); [11] F. de Leeuw (pers. comm.); [12] Barrett & Berge (1996); [13] Lide (1993); [14] personal assessment

Table B.3: Substance-specific input parameters for non-aromatics

Compound name	Unit	acrylonitrile	acrolein	1,3-butadiene	carbon disulfide	ethylene	formaldehyde	propylene oxide	Source
CAS nr.	-	107-13-1	107-02-8	106-99-0	75-15-0	74-85-1	50-00-0	75-56-9	
Effects assessment									1-8
oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$1.0 \cdot 10^{-12}$	$5.0 \cdot 10^{-9}$				$1.5 \cdot 10^{-7}$	$2.9 \cdot 10^{-12}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$5.0 \cdot 10^{-11}$	$5.0 \cdot 10^{-10}$	$4.0 \cdot 10^{-12}$	$1.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-7}$	$9.0 \cdot 10^{-10}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$7.6 \cdot 10^{-6}$	$7.0 \cdot 10^{-9}$	$7.1 \cdot 10^{-5}$	$2.1 \cdot 10^{-6}$	$8.5 \cdot 10^{-3}$	$2.1 \cdot 10^{-6}$	$1.7 \cdot 10^{-4}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	
Physico-chemical properties									9-15
molecular weight	$g.mol^{-1}$	53.06	56.04	54.09	76.12	28.054	30.03	58.08	
octanol-water partition coefficient	$m^3.m^{-3}$	1.8	0.1	97.7	87	13.5	2.2	1.1	
melting point	°C	-83.55	-87	-108.9	-111.2	-169.14	-92	-112.13	
vapor pressure (25 °C)	Pa	$1.1 \cdot 10^{4}$	$3.65 \cdot 10^{4}$	$2.8 \cdot 10^{5}$	$4.9 \cdot 10^{4}$	$2.7 \cdot 10^{9}$	$4.5 \cdot 10^{5}$	$7.1 \cdot 10^{4}$	
solubility (25 °C)	$mg.l^{-1}$	$7.55 \cdot 10^{4}$	$2.08 \cdot 10^{5}$	735	2400	260	$1.22 \cdot 10^{6}$	$4.76 \cdot 10^{5}$	
Partition coefficients									9, 10, 16, 17
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$	11.1	2.4	$2.57 \cdot 10^{5}$			$3.2 \cdot 10^{-2}$	8.5	
organic carbon partition coefficient	$l.kg^{-1}$		0.5	129					
Degradation rates									13, 18-23
reaction half-life in air	d	4.95			9		0.15	30.9	
hydroxyl radical reaction in air (-10 °C)	$cm^3.molec^{-1}.sec^{-1}$		$2.2 \cdot 10^{-11}$	$8.2 \cdot 10^{-11}$		$1.0 \cdot 10^{-11}$			
hydroxyl radical reaction in air (12 °C)	$cm^3.molec^{-1}.sec^{-1}$		$2.0 \cdot 10^{-11}$	$7.2 \cdot 10^{-11}$		$9.1 \cdot 10^{-12}$			
hydroxyl radical reaction in air (25 °C)	$cm^3.molec^{-1}.sec^{-1}$		$1.9 \cdot 10^{-11}$	$6.7 \cdot 10^{-11}$		$8.5 \cdot 10^{-12}$			
hydrolysis in water, soil, sediment (pH=6; 12 °C)	d							13	
hydrolysis in water, soil, sediment (pH=7; 12 °C)	d							14	
hydrolysis in water, soil, sediment (pH=8; 12 °C)	d							14	
biodegradation in surface water (12C)	d	9.4	24.4	24.4	30	9.2	4.6	30	
biodegradation in soil (12 °C)	d	9.4	24.4	24.4	100	9.2	4.6	100	
aerobic biodegradation in the sediment zone (12 °C)	d	9.4	24.4	24.4	100	9.2	4.6	100	
anaerobic biodegradation in the sediment zone (12 °C)	d	37.4	101	97	400	36.9	18.5	400	
Exposure assessment									19, 24-27
bioconcentration factor in fish	$l.kg(wwt)^{-1}$		344						
bioavailability for inhalation	-	0.95	0.82	0.65			1	1	
bioavailability for oral uptake	-	0.98							

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] WHO-EURO (1987); [2] WHO-EURO (1996); [3] Janus et al. (1994); [4] RIZA (1999); [5] Environmental Defense Fund (1999); [6] Huijbregts (1999); [7] USEPA (1998b); [8] Janssen et al. (1995); [9] Mackay et al. (1993); [10] Mackay et al. (1995); [11] Mackay et al. (1997); [12] Cambridgesoft Corporation (1998); [13] Howard (1989); [14] Environmental Science Center (1998); [15] Verschueren (1996); [16] Lide (1993); [17] Bockting et al. (1993); [18] Howard et al. (1991); [19] Slooff (1988); [20] Jager et al. (1997); [21] RIVM et al. (1998); [22] Howard (1990); [23] Atkinson (1986); [24] WHO (1989c); [25] Slooff et al. (1991c); [26] WHO (1992); [27] Owen (1990)

Table B.4a: Substance-specific input parameters for aromatics

Compound name	Unit	Benzene	Toluene	Styrene	Phenol	Ethylbenzene	m-xylene	o-xylene	p-xylene	Butylbenzyl-phtalate	Source
CAS nr.	-	71-43-2	108-88-3	100-42-5	108-95-2	100-41-4	108-38-3	95-47-6	106-42-3	85-68-7	
Effects assessment											1-8
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$1.0 \cdot 10^{-7}$	$2.0 \cdot 10^{-7}$	$7.7 \cdot 10^{-8}$	$6.0 \cdot 10^{-8}$	$1.36 \cdot 10^{-7}$	$1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	$2.0 \cdot 10^{-7}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$1.67 \cdot 10^{-10}$	$2.6 \cdot 10^{-7}$	$2.6 \cdot 10^{-7}$	$6.0 \cdot 10^{-7}$	$7.7 \cdot 10^{-8}$	$1.0 \cdot 10^{-6}$	$3.4 \cdot 10^{-7}$	$1.0 \cdot 10^{-6}$	$5.0 \cdot 10^{-8}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.4 \cdot 10^{-3}$	$7.3 \cdot 10^{-4}$	$5.7 \cdot 10^{-4}$	$9.0 \cdot 10^{-7}$	$3.7 \cdot 10^{-4}$	$3.3 \cdot 10^{-4}$	$4.0 \cdot 10^{-4}$	$4.0 \cdot 10^{-4}$	$7.5 \cdot 10^{-6}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	$1.5 \cdot 10^{-7}$	EP[a]	$5.6 \cdot 10^{-8}$	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	
Physico-chemical properties											10-13
molecular weight	$g.mol^{-1}$	78.11	92.13	104.14	94.1	106.2	106.2	106.2	106.2	312.39	
octanol-water partition coefficient	$m^3.m^{-3}$	147	490	1122	29	1349	1585	1413	1514	56234	
melting point	°C	5.53	-95	-30.6	41	-95	-47.9	-25.2	13.2	-35	
vapor pressure (25 °C)	Pa	$1.3 \cdot 10^{4}$	$3.8 \cdot 10^{3}$	800	47	$1.3 \cdot 10^{3}$	$1.1 \cdot 10^{3}$	$1.2 \cdot 10^{3}$	$1.2 \cdot 10^{3}$	$8.6 \cdot 10^{-4}$	
solubility (25 °C)	$mg.l^{-1}$	1752	515	300	88360	152	160	220	215	2.7	
Partition coefficients											9, 10, 14-16
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$	$5.9 \cdot 10^{2}$	$9.2 \cdot 10^{2}$	$2.8 \cdot 10^{2}$	$4.0 \cdot 10^{-2}$	$8.1 \cdot 10^{2}$	$9.9 \cdot 10^{2}$	$6.8 \cdot 10^{2}$	$1.0 \cdot 10^{3}$		
organic carbon partition coefficient	$l.kg^{-1}$	79	115	912	35	166	218	189	525	1622	
Degradation rates											17-19
reaction half-life in air	d			0.3	0.6	2.1		1.1	1.1	1.5	
hydroxyl radical reaction in air (-10 °C)	$cm^3.molec^{-1}.sec^{-1}$	$1.1 \cdot 10^{-12}$	$7.1 \cdot 10^{-12}$				$2.6 \cdot 10^{-11}$				
hydroxyl radical reaction in air (12 °C)	$cm^3.molec^{-1}.sec^{-1}$	$1.2 \cdot 10^{-12}$	$6.5 \cdot 10^{-12}$				$2.5 \cdot 10^{-11}$				
hydroxyl radical reaction in air (25 °C)	$cm^3.molec^{-1}.sec^{-1}$	$1.2 \cdot 10^{-12}$	$6.2 \cdot 10^{-12}$				$2.5 \cdot 10^{-11}$				
biodegradation in surface water (12 °C)	d	16	16	35	2	10	24	24	24	5	
biodegradation in soil (12 °C)	d	331	16	35	6	10	24	24	24	5	
aerobic biodegradation in sediment (12 °C)	d	16	16	35	2	10	24	24	24	5	
anaerobic biodegradation in sediment (12 °C)	d	495	189	138	26	349	98	444	98	124	
Exposure assessment											10-13, 20-26
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	6	8	14	17	16	19	17	19	12	
plant conductance	$m.s^{-1}$				$7.56 \cdot 10^{-4}$						
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$	2.9									
bioavailability for inhalation	-	0.47	0.5		0.75	0.64	0.64	0.64	0.64		
bioavailability for oral uptake	-	1	1		0.95	0.82	1	1	1	0.5	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] WHO-EURO (1996); [2] Environmental Defense Fund (1999); [3] Rademaker et al. (1993); [4] Janus et al. (1994); [5] Vermeire et al. (1991); [6] USEPA (1998b); [7] RIZA (1999); [8] Huijbregts (1999); [9] Van de Plassche & Bockting (1993); [10] Mackay et al. (1992a); [11] Mackay et al. (1993); [12] Mackay et al. (1995);); [13] Staples et al. (1997); [14] Lide (1993); [15] Sabljic et al. (1995); [16] Bockting et al. (1993); [17] Howard et al. (1991); [18] RIVM et al. (1998); [19] Atkinson (1986); [20] Nendza (1991); [21] Devillers et al. (1996); [22] Owen (1990); [23] WHO (1994b); [24] WHO (1996c); [25] Peijnenburg et al. (1991); [26] Riederer (1995)

Table B.4b: Substance-specific input parameters for aromatics

Compound name	Unit	Di(2-ethylhexyl)-phtalate	Dibutyl-phtalate	Diethyl-phtalate	Dihexyl-phtalate	Diisooctyl-phtalate	Diisodecyl-phtalate	Dimethyl-phtalate	Dioctyl-phtalate	Phtalic anhydride	Source
CAS nr.	-	117-81-7	84-74-2	84-66-2	84-75-3	27554-26-3	26761-40-0	133-11-3	117-84-0	85-44-9	
Effects assessment											1-7
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$2.5 \cdot 10^{-8}$	$1.0 \cdot 10^{-7}$	$8.0 \cdot 10^{-7}$	[a] $1.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-8}$	$5.0 \cdot 10^{-8}$	[a] $1.0 \cdot 10^{-9}$	$2.0 \cdot 10^{-8}$	$3.75 \cdot 10^{-7}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$1.0 \cdot 10^{-8}$			[a] $4.7 \cdot 10^{-9}$			[a] $4.7 \cdot 10^{-9}$		$1.0 \cdot 10^{-8}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.6 \cdot 10^{-6}$	$1.0 \cdot 10^{-5}$	$7.3 \cdot 10^{-5}$	$8.4 \cdot 10^{-6}$	$1.2 \cdot 10^{-6}$	$2.9 \cdot 10^{-6}$	$1.9 \cdot 10^{-4}$	$6.4 \cdot 10^{-6}$	$7.8 \cdot 10^{-6}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP [b]	EP [b]	$5.0 \cdot 10^{-9}$	EP [b]	EP [b]	EP [b]	$1.5 \cdot 10^{-9}$	EP [b]	EP [b]	
Physico-chemical properties											8-12
molecular weight	$g.mol^{-1}$	390.54	278.35	222.26	334.5	390.6	446.7	194.2	390.6	148.11	
octanol-water partition coefficient	$m^3.m^{-3}$	2018366	38459	266	3427678	100000000	100000000	73	114815362	40	
melting point	°C	-47	-35	-40.5	-27.4	-46	-46	5	-25	130.8	
vapor pressure (25 °C)	Pa	$1.3 \cdot 10^{-5}$	$2.7 \cdot 10^{-3}$	$8.2 \cdot 10^{-2}$	$6.7 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$6.7 \cdot 10^{-5}$	$2.5 \cdot 10^{-1}$	$1.3 \cdot 10^{-5}$	$3.8 \cdot 10^{-2}$	
solubility (25 °C)	$mg.l^{-1}$	0.003	11.2	1090	0.05	0.001	0.001	4100	0.0005	6200	
Partition coefficients											12-15
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$		$4.6 \cdot 10^{-2}$	$4.8 \cdot 10^{-2}$				$1.1 \cdot 10^{-2}$		$6.2 \cdot 10^{-4}$	
organic carbon partition coefficient	$l.kg^{-1}$	275423	1380	537	52481		213796	214		36	
Degradation rates											16-19
reaction half-life in air	d	0.7	1.9	5.3	1.6	1.6	1.6	28.0	1.1	121	
hydrolysis in water, soil, sediment (pH=6; 12 °C)	d							$2 \cdot 10^{4}$		$5 \cdot 10^{-3}$	
hydrolysis in water, soil, sediment (pH=7; 12 °C)	d							$2 \cdot 10^{3}$		$3 \cdot 10^{-2}$	
hydrolysis in water, soil, sediment (pH=8; 12 °C)	d							23		$5 \cdot 10^{-2}$	
biodegradation in surface water (12 °C)	d	19	7	23	35	27	27	5	24	5	
biodegradation in soil (12 °C)	d	19	12	23	60	47	47	5	24	5	
aerobic biodegradation in sediment (12 °C)	d	19	8	23	60	47	47	5	24	5	
anaerobic biodegradation in sediment (12 °C)	d	223	12	138	1092	853	853	18	447	18	
metabolism in plant tissue	d	4									
Exposure assessment											8, 9, 20, 21
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	300	167	117		92	10	11			
plant conductance	$m.s^{-1}$	$4.03 \cdot 10^{-4}$									
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$		0.002								
bioavailability for oral uptake	-	0.5	0.85	0.5	0.5	0.5	0.5	0.5	0.5		

[a] Default values for HLV_{oral} and HLV_{inh}, as proposed by RIVM et al. (1994); [b] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] Janus et al. (1994); [2] USEPA (1998b); [3] Environmental Defense fund (1999); [4] Guinée et al. (1996a); [5] Vermeire et al. (1991); [6] RIZA (1999); [7] Huijbregts (1999); [8] Mackay et al. (1995); [9] Staples et al. (1997); [10] USEPA (1998a); [11] Howard (1989); [12] Sabljic et al. (1995); [13] Bockting et al. (1993); [14] Lide (1993); [15] Slooff (1994); [16] Howard et al. (1991); [17] RIVM et al. (1998); [18] Komoßa et al. (1995); [19] Peijnenburg et al. (1991); [20] Owen (1990); [21] Riederer (1995)

Table B.5: Substance-specific input parameters for polycyclic aromatics

Compound name	Unit	Naphthalene	Anthracene	Phenanthrene	Fluoranthene	Benzo[a]-anthracene	Chrysene	Benzo[k]-fluoranthene	Benzo[a]-pyrene	Benzo[ghi]-perylene	Indeno[1,2,3-cd]pyrene	Carcinogic PAH (total)	Source
CAS nr.	-	91-20-3	120-12-7	85-01-8	206-44-0	56-55-3	218-01-9	207-08-9	50-32-8	191-24-2	193-39-5		
Effect assessment													1-5
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$5.0 \cdot 10^{-8}$	$3.0 \cdot 10^{-7}$									$6.3 \cdot 10^{-11}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$3.0 \cdot 10^{-9}$										$1.2 \cdot 10^{-14}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$4.2 \cdot 10^{-7}$	$3.34 \cdot 10^{-8}$	$3.2 \cdot 10^{-6}$	$2.4 \cdot 10^{-7}$	$1.0 \cdot 10^{-8}$	$3.4 \cdot 10^{-7}$	$3.6 \cdot 10^{-9}$	$5.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-8}$	$1.8 \cdot 10^{-8}$	$1.15 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	EP[a]	EP[a]	EP[a]	$7.0 \cdot 10^{-9}$	EP[a]	EP[a]	$8.0 \cdot 10^{-9}$	EP[a]	EP[a]	$9.5 \cdot 10^{-8}$	
Physico-chemical properties													2, 6-10
molecular weight	$g.mol^{-1}$	128.19	178.2	178.2	202.3	228.3	228.3	252.32	252.3	268.36	276.34	239	
octanol-water partition coefficient	$m^3.m^{-3}$	2344	34674	37154	165959	812830	316228	1000000	1817730	3162278	3837072	1142279	
melting point	°C	80.5	216.2	101	111	160	255	217	175	277	162.5	195.6	
vapor pressure (25 °C)	Pa	10.4	$1.0 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	$1.2 \cdot 10^{-3}$	$2.8 \cdot 10^{-5}$	$5.7 \cdot 10^{-7}$	$5.2 \cdot 10^{-8}$	$7.1 \cdot 10^{-7}$	$1.4 \cdot 10^{-8}$	$1.3 \cdot 10^{-8}$	$2.5 \cdot 10^{-4}$	
solubility (25 °C)	$mg.l^{-1}$	31	0.045	1.1	0.26	$1.1 \cdot 10^{-2}$	$2.0 \cdot 10^{-3}$	$8.0 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$2.6 \cdot 10^{-4}$	$6.2 \cdot 10^{-2}$	$5.9 \cdot 10^{-2}$	
Partition coefficients													7, 11-13
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$	49							$9.2 \cdot 10^{-2}$			$6.8 \cdot 10^{-3}$	
organic carbon partition coefficient	$l.kg^{-1}$	933	23988	22387	41687	199526						107000	
Degradation rates													7, 14-18
reaction half-life in air	d		1.23	1.26	0.5	0.07	0.2	0.3	0.035	008	0.16	0.25	
hydroxyl radical reaction in air (-10 °C)	$cm^3.molec^{-1}.sec^{-1}$	$3.2 \cdot 10^{-11}$											
hydroxyl radical reaction in air (12 °C)	$cm^3.molec^{-1}.sec^{-1}$	$2.5 \cdot 10^{-11}$											
hydroxyl radical reaction in air (25 °C)	$cm^3.molec^{-1}.sec^{-1}$	$2.7 \cdot 10^{-11}$											
biodegradation in surface water (12 °C)	d	6	264	99	433	459	1062	2434	303	1080	1154	1271	
biodegradation in soil (12 °C)	d	49	264	99	433	459	1062	2434	387	1080	1154	1276	
aerobic biodegradation in sediment (12 °C)	d	6	264	99	433	459	1062	2434	303	1080	1154	1271	
anaerobic biodegradation in sediment (12 °C)	d	140	1058	394	1731	1837	4249	9735	1213	4320	4617	5082	
metabolism in plant tissue	d								1.8				
Exposure assessment													6, 7, 19-23
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	398	912	2630		10000			312			18565	
bioconcentration factor from porewater to roots	$l.kg\ (wwt)^{-1}$	30		2700	65								
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$								0.015				
bioavailability for inhalation	-								0.29			0.29	
bioavailability for oral uptake	-	1							0.5			0.5	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning;[1] Vermeire (1993); [2] WHO-EURO (1996); [3] USEPA (1998b); [4] RIZA (1999); [5] Huijbregts (1999); [6] Mackay et al. (1992b); [7] McKone et al., 1995); [8] Cambridgesoft Corporation (1998); [9] Spectrum Laboratories (1998); [10] Environmental Science Center, 1998; [11] Lide (1993); [12] Sabljic et al. (1995); [13] Bockting et al. (1993); [14] Howard et

al. (1991); [15] RIVM et al. (1998); [16] Atkinson (1986); [17] Kwok et al. (1994); [18] Komoßa et al. (1995); [19] Nendza (1991); [20] Devillers et al. (1996); [21] Polder et al. (1995); [22] Dowdy & McKone (1997); [23] Owen (1990)

Table B.6: Substance-specific input parameters for halogenated non-aromatics

Compound name	Unit	dichloro-methane	trichloro-methane	tetrachloro-methane	1,2-dichloro-ethane	1,1,1-trichloro-ethane	trichloro-ethylene	tetrachloro-ethylene	vinyl-chloride	hexachloro-butadiene	Source
CAS nr.	-	75-09-2	67-66-3	56-23-5	107-06-2	71-55-6	79-01-6	127-18-4	75-01-4	87-68-3	
Effects assessment											1-8
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$6.0 \cdot 10^{-8}$	$1.5 \cdot 10^{-8}$	$4.0 \cdot 10^{-9}$	$1.4 \cdot 10^{-10}$		$5.4 \cdot 10^{-7}$	$1.6 \cdot 10^{-8}$	$3.51 \cdot 10^{-11}$	$2.0 \cdot 10^{-10}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$4.5 \cdot 10^{-7}$	$1.0 \cdot 10^{-7}$	$6.0 \cdot 10^{-8}$	$7.0 \cdot 10^{-7}$	$3.8 \cdot 10^{-7}$	$5.39 \cdot 10^{-9}$	$2.5 \cdot 10^{-7}$	$1.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-11}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.0 \cdot 10^{-2}$	$5.9 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$1.4 \cdot 10^{-2}$	$2.1 \cdot 10^{-3}$	$2.4 \cdot 10^{-3}$	$3.3 \cdot 10^{-4}$	$8.2 \cdot 10^{-3}$	$5.0 \cdot 10^{-9}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	$4.6 \cdot 10^{-8}$	EP[a]	EP[a]	
Physico-chemical properties											9, 10
molecular weight	$g.mol^{-1}$	84.94	119.38	153.82	98.96	133.41	131.39	165.83	62.5	260.76	
octanol-water partition coefficient	$m^3.m^{-3}$	17.8	93.3	436.5	28	309	309	377	24	50119	
melting point	°C	-95	-63.5	-22.9	-35.36	-30.41	-83.5	-19	-153.8	-21	
vapor pressure (25 °C)	Pa	26222	26244	15250	10740	16500	9664	2560	354600	20	
solubility (25 °C)	$mg.l^{-1}$	13200	8200	800	8514	1495	1437	257	2763	3.2	
Partition coefficients											9-13
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$	285.7	413.3	3248.3	117	2015	1028	1742	2192.8		
organic carbon partition coefficient	$l.kg^{-1}$	36	65	34	42	66.1	110	240			
Degradation rates											9, 10, 14-17
reaction half-life in air	d			4000	73,2				2.4	716	
hydroxyl radical reaction in air (-10 °C)	$cm^3..molec^{-1}.sec^{-1}$	$8.8 \cdot 10^{-14}$	$6.4 \cdot 10^{-14}$			$5.6 \cdot 10^{-15}$	$2.8 \cdot 10^{-12}$	$9.7 \cdot 10^{-14}$			
hydroxyl radical reaction in air (12 °C)	$cm^3.molec^{-1}.sec^{-1}$	$1.2 \cdot 10^{-13}$	$8.7 \cdot 10^{-14}$			$9.2 \cdot 10^{-15}$	$2.5 \cdot 10^{-12}$	$1.4 \cdot 10^{-13}$			
hydroxyl radical reaction in air (25 °C)	$cm^3..molec^{-1}.sec^{-1}$	$1.4 \cdot 10^{-13}$	$1.0 \cdot 10^{-13}$			$1.2 \cdot 10^{-14}$	$2.4 \cdot 10^{-12}$	$1.7 \cdot 10^{-13}$			
hydrolysis in water, soil, sediment (pH=6, 7, 8; 12 °C)	d			14600	4379	382	560				
biodegradation in surface water (12 °C)	d	24	124	429	435	341	104	122	124	124	
biodegradation in soil (12 °C)	d	24	124	429	102	341	601	444	124	124	
aerobic biodegradation in the sediment zone (12 °C)	d	24	124	429	234	341	313	569	124	124	
anaerobic biodegradation in the sediment zone (12 °C)	d	98	24	24	936	1364	702	702	495	495	
Exposure assessment											9, 10, 18-23
bioconcentration factor in fish	$l.kg(wwt)^{-1}$		4	30	2	9	26	44	1	9886	
bioavailability for inhalation	-		0.7	0.6			0.6		0.64		
bioavailability for oral uptake	-		0.5	0.9							

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] Vermeire et al. (1991); [2] WHO-EURO (1987); [3] WHO-EURO (1996); [4] USEPA (1998b); [5] Janssen et al. (1995); [6] Janus et al. (1994); [7] RIZA (1999); [8] Huijbregts (1999); [9] Mackay et al. (1993); [10] McKone et al. (1995); [11] Bockting et al. (1993); [12] Van de Plassche & Bockting (1993); [13] Lide (1993); [14] Howard et al. (1991); [15] RIVM et al. (1998); [16] Jeffers et al. (1996); [17] Atkinson (1986); [18] Devillers et al. (1996); [19] Nendza (1991); [20] WHO (1994c); [21] RIVM & TNO (1986); [22] WHO (1985a); [23] Owen (1990)

Table B.7a: Substance-specific input parameters for halogenated aromatics

Compound name	Unit	chloro-benzene	1,2-dichloro-benzene	1,3-dichloro-benzene	1,4-dichloro-benzene	1,2,3-trichloro-benzene	1,2,4-trichloro-benzene	1,3,5-trichloro-benzene	1,2,3,4-tetrachloro-benzene	Source
CAS nr.	-	108-90-7	95-50-1	541-73-1	106-46-7	87-61-6	120-82-1	108-70-3	634-66-2	
Effects assessment										1-5
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.0 \cdot 10^{-7}$	$6.0 \cdot 10^{-7}$	[a] $1.0 \cdot 10^{-9}$	$2.0 \cdot 10^{-7}$	$2.0 \cdot 10^{-8}$	$2.0 \cdot 10^{-8}$	$2.0 \cdot 10^{-8}$	$4.0 \cdot 10^{-9}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$4.2 \cdot 10^{-8}$	$6.0 \cdot 10^{-8}$	[a] $4.7 \cdot 10^{-9}$	$6.7 \cdot 10^{-7}$	$4.0 \cdot 10^{-9}$	$4.0 \cdot 10^{-9}$	$4.0 \cdot 10^{-9}$		
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$6.9 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$	$2.1 \cdot 10^{-4}$	$2.6 \cdot 10^{-4}$	$6.4 \cdot 10^{-5}$	$7.9 \cdot 10^{-5}$	$5.7 \cdot 10^{-5}$	$2.3 \cdot 10^{-5}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$1.8 \cdot 10^{-7}$	EP[b]	EP[b]	$9.4 \cdot 10^{-8}$	$4.3 \cdot 10^{-9}$	$3.8 \cdot 10^{-8}$	$1.5 \cdot 10^{-7}$	$6.9 \cdot 10^{-8}$	
Physico-chemical properties										6, 7
molecular weight	$g.mol^{-1}$	112.6	147.01	147.01	147.01	181.45	181.45	181.45	215.9	
octanol-water partition coefficient	$m^3.m^{-3}$	631	2512	2512	2925	12589	12589	12589	31623	
melting point	°C	-45.6	-17	-24.9	53.1	53	16.95	64	47.5	
vapor pressure (25 °C)	Pa	1580	196	307	149	28	61	32	5.2	
solubility (25 °C)	$mg.l^{-1}$	484	118	120	72	21	40	5.3	7.8	
Partition coefficients										6-11
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$	454	219	305	297	306	207	175	70.5	
organic carbon partition coefficient	$l.kg^{-1}$	219	316	302	519	1950	1778	933	9120	
Degradation rates										7, 12, 13
reaction half-life in air	d	18.2	38.2	22.3	50.2	32.1	32.1	32.1	190.8	
biodegradation in surface water (12 °C)	d	176	124	124	124	124	124	124	124	
biodegradation in soil (12 °C)	d	176	782	782	782	124	124	124	124	
aerobic biodegradation in sediment (12 °C)	d	176	124	124	124	124	124	124	124	
anaerobic biodegradation in sediment (12 °C)	d	704	513	513	495	495	495	495	513	
Exposure assessment										6, 7, 14-15
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	74	186	154	196	1778	2239	2042	4074	
partitioning coefficient between leaves and air	$m^3.m^{-3}$				75.5		1050			
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$				0.34	0.07	0.07	0.07	0.12	

[a] Default values for HLV_{oral} and HLV_{inh}, as proposed by RIVM et al. (1994); [b] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] Vermeire et al. (1991); [2] Rademaker et al. (1993); [3] Janus et al. (1994); [4] RIZA (1999); [5] Huijbregts (1999); [6] Mackay et al. (1992a); [7] McKone et al. (1995); [8] Van de Plassche & Bockting (1993); [9] Sabljic et al. (1995); [10] Bockting et al. (1993); [11] Lide (1993); [12] Howard et al. (1991); [13] RIVM et al. (1998); [14] Polder et al. (1998); [15] Dowdy & McKone (1997)

Table B.7b: Substance-specific input parameters for halogenated aromatics

Compound name	Unit	1,2,3,5-tetra-chlorobenzene	1,2,4,5-tetra-chlorobenzene	pentachloro-benzene	hexachloro-benzene	2-chloro-phenol	2,4-dichloro-phenol	2,4,5-tri-chlorophenol	2,4,6-tri-chlorophenol	Source
CAS nr.	-	634-90-2	95-94-3	608-93-5	118-74-1	95-57-8	120-83-2	95-95-4	88-06-2	
Effects assessment										1-6
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$4.0 \cdot 10^{-9}$	$4.0 \cdot 10^{-9}$	$8.0 \cdot 10^{-10}$	$5.7 \cdot 10^{-13}$	$5.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-7}$	$8.6 \cdot 10^{-11}$	
Inhalatory Human Limit Value	$kg.m^{-3}$				$2.0 \cdot 10^{-12}$	$1.8 \cdot 10^{-8}$			$3.0 \cdot 10^{-10}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.2 \cdot 10^{-5}$	$2.6 \cdot 10^{-5}$	$7.5 \cdot 10^{-6}$	$2.4 \cdot 10^{-6}$	$3.0 \cdot 10^{-6}$	$5.8 \cdot 10^{-6}$	$4.8 \cdot 10^{-6}$	$1.3 \cdot 10^{-5}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$3.5 \cdot 10^{-9}$	$3.0 \cdot 10^{-9}$	$8.3 \cdot 10^{-8}$	EP[a]	EP[a]	EP[a]	$2.3 \cdot 10^{-8}$	$2.6 \cdot 10^{-8}$	
Physico-chemical properties										7-9
molecular weight	$g.mol^{-1}$	215.9	215.9	250.3	284.79	128.56	163	197.45	197.45	
octanol-water partition coefficient	$m^3.m^{-3}$	31623	31623	100000	316228	148	1589	5273	4921	
melting point	°C	54.5	140	86	228	9	44	69	69.5	
vapor pressure (25 °C)	Pa	9.8	0,7	$2.2 \cdot 10^{-1}$	$2.3 \cdot 10^{-3}$	132	12	2.5	1.25	
solubility (25 °C)	$mg.l^{-1}$	3.6	1.3	0.65	$5.0 \cdot 10^{-3}$	24650[b]	4500[b]	948[b]	434[b]	
dissociation constant	-					8.49	7.68	7.43	7.42	
Partition coefficients										10-13
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$	118	94	$7.05 \cdot 10^{1}$	78.2	$5.7 \cdot 10^{-2}$			$6.2 \cdot 10^{-3}$	
organic carbon partition coefficient	$l.kg^{-1}$	2399	8128	4169	10965	136	295	1413	1047	
Degradation rates										7, 14-16
reaction half-life in air	d	190.8	190.8	271.9	938.3	2.0	5.3	7.6	30.8	
biodegradation in surface water (12 °C)	d	124	124	451	2481	53	8	220	39	
biodegradation in soil (12 °C)	d	124	124	451	2481	6	39	220	39	
aerobic biodegradation in sediment (12 °C)	d	124	124	451	2481	53	8	220	39	
anaerobic biodegradation in sediment (12 °C)	d	513	513	1805	9925	212	42	836	967	
metabolism in plant tissue	d				10.2					
Exposure assessment										7, 8, 17-22
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	2042	6095	5754	13490	214		1905	676	
partitioning coefficient between leaves and air	$m^3.m^{-3}$		$2.4 \cdot 10^{3}$	$1.5 \cdot 10^{4}$	$2.0 \cdot 10^{4}$					
plant conductance	$m.s^{-1}$				$6.76 \cdot 10^{-4}$					
bioconcentration factor from porewater to roots	$l.kg\ (wwt)^{-1}$						130			
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$	0.12	0.12	0.05	0.03		0.09			
biotransfer factor for meat	$d.kg^{-1}$				0.05					
biotransfer factor for milk	$d.kg^{-1}$				0.009					

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [1] Vermeire et al. (1991); [2] Environmental Defense Fund (1999); [3] USEPA (1998); [4] Janus et al. (1994); [5] RIZA (1999); [6] Huijbregts (1999); [7] Mackay et al. (1992a); [8] Mackay et al. (1997); [9] Mackay et al. (1995); [10] Van de Plassche & Bockting (1993); [11] Sabljic et al. (1995); [12] Bockting et al. (1993); [13] Lide (1993); [14] Howard et al. (1991); [15] RIVM et al. (1998); [16] Komoßa et al. (1995); [17] Nendza (1991); [18] Polder et al. (1995); [19] Polder et al. (1998); [20] Dowdy & McKone (1997); [21] Travis & Arms (1988); [22] Riederer (1995)

Table B.7c: Substance-specific input parameters for halogenated aromatics

Compound name	Unit	2,3,4,6-tetra-chlorophenol	pentachloro-phenol	Benzyl-chloride	3-chloro-aniline	4-chloro-aniline	3,4-chloro-aniline	1-chloro-4-nitrobenzene	pentachloro-nitrobenzene	2,3,7,8-TCDD	Source
CAS nr.	-	58-90-2	87-86-5	100-44-7	108-42-9	106-47-8	95-76-1	100-00-5	82-68-8	1746-01-6	
Effects assessment											1-10
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.0 \cdot 10^{-8}$	$3.0 \cdot 10^{-8}$	$5.7 \cdot 10^{-12}$	$9.0 \cdot 10^{-12}$	$9.0 \cdot 10^{-12}$	$2.0 \cdot 10^{-9}$	$5.56 \cdot 10^{-11}$	$7.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-15}$	
Inhalatory Human Limit Value	$kg.m^{-3}$		$1.0 \cdot 10^{-7}$		$4.0 \cdot 10^{-11}$	$4.0 \cdot 10^{-11}$					
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$1.4 \cdot 10^{-6}$	$3.5 \cdot 10^{-6}$	$1.3 \cdot 10^{-6}$	$1.3 \cdot 10^{-6}$	$8.0 \cdot 10^{-7}$	$8.0 \cdot 10^{-7}$	$3.2 \cdot 10^{-6}$	$2.9 \cdot 10^{-7}$	$1.2 \cdot 10^{-12}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	$1.1 \cdot 10^{-8}$	EP[a]	$3.1 \cdot 10^{-8}$	EP[a]	$1.5 \cdot 10^{-8}$	EP[a]	EP[a]	EP[a]	
Physico-chemical properties											10-15
molecular weight	$g.mol^{-1}$	231.89	266.34	126.58	127.57	127.57	162.06	157.56	295.3	322	
octanol-water partition coefficient	$m^3.m^{-3}$	42975	282026	200	76	68	468	245	44000	$8.13 \cdot 10^{6}$	
melting point	°C	70	190	-45.5	-10	70	71.5	83	146	305	
vapor pressure (25 °C)	Pa	$2.8 \cdot 10^{-1}$	$4.15 \cdot 10^{-3}$	163.7	9.5	2.3	1.3	2.0	$6.6 \cdot 10^{-3}$	$2.0 \cdot 10^{-7}$	
solubility (25 °C)	$mg.l^{-1}$	183[b]	14[b]	528	5440[b]	3000[b]	92[b]	342	0.44	$2.5 \cdot 10^{-5}$	
dissociation constant	-	5.38	4.92		3.5	4.0	2.5				
Partition coefficients											9, 15-18
Henry's law constant (25 °C)	$Pa.m^{-3}.mol^{-1}$					1.1		3.6			
organic carbon partition coefficient	$l.kg^{-1}$	2239	32359		355	180	977		23000	$1.8 \cdot 10^{6}$	
Degradation rates											11, 14, 19-25
reaction half-life in air	d	25	34.8	5.5	0.2	0.2	0.4	272	2198		
hydroxyl radical reaction in air (-10 °C)	$cm^3..molec^{-1}.sec^{-1}$									$4.0 \cdot 10^{-13}$	
hydroxyl radical reaction in air (12 °C)	$cm^3..molec^{-1}.sec^{-1}$									$6.6 \cdot 10^{-13}$	
hydroxyl radical reaction in air (25 °C)	$cm^3..molec^{-1}.sec^{-1}$									$8.6 \cdot 10^{-13}$	
hydrolysis in water, soil, sediment (PH=6, 7, 8; 12 °C)	d			5							
biodegradation in surface water (12 °C)	d	120	112	24	30	30	1000	451	673	622	
biodegradation in soil (12 °C)	d	120	112	24	100	100	1000	451	673	3194	
aerobic biodegradation in sediment (12 °C)	d	120	112	24	100	100	1000	451	673	622	
anaerobic biodegradation in sediment (12 °C)	d	478	441	98	400	400	4000	1805	31	1757	
metabolism in plant tissue	d					0.6	0.7				
photodegradation upon plant tissue	d									6.2	
Exposure assessment											14, 15, 26-32
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	447	268		4	5	30		201	12314	
partitioning coefficient between leaves and air	$m^3.m^{-3}$									$3.2 \cdot 10^{7}$	
plant conductance	$m.s^{-1}$		$1.91 \cdot 10^{-3}$								
transpiration stream concentration factor	-	0.04[c]	0.04[c]		0.04[c]	0.04[c]	0.04[c]				
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$	0.7[c]	1.2		0.7[c]	0.7[c]	0.7[c]			780	
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$						0.35			$3 \cdot 10^{-2}$	
biotransfer factor for meat									$1.8 \cdot 10^{-3}$	0.11	
biotransfer factor for milk	$d.kg^{-1}$								$1.6 \cdot 10^{-4}$	$8 \cdot 10^{-3}$	
bioavailability for oral uptake	-									0.5	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [c] assumed default value for dissociating acids at environmental pH of 7, based on Briggs et al. (1987); [1] USEPA (1998b); [2] Vermeire et al. (1991); [3] Environmental Defense Fund (1999); [4] Janssen et al. (1998); [5] Janus et al. (1994); [6] Health Council of the Netherlands (1996); [7] Lu (1995); [8] RIZA (1999); [9] Huijbregts (1999); [10] Guinée et al. (1996a); [11] Howard (1989); [12] Verschueren (1996); [13] Mackay et al. (1992b); [14] Mackay et al. (1995); [15] Mackay et al. (1997); [16] Sabljic et al. (1995); [17] Bockting et al. (1993); [18] Lide (1993); [19] Howard et al. (1991); [20] RIVM et al. (1998); [21] Jager et al. (1997); [22] Syraceuse Research Corporation (1993);[23] Brubaker & Hites (1997); [24] Trapp & Matthies (1995); [25] Komoßa et al. (1995); [26] Liem et al. (1993); [27] Polder et al. (1995); [28] Polder et al. (1998); [29] Dowdy et al. (1996); [30] Dowdy & McKone (1997); [31] WHO (1989a); [32] Riederer (1995)

Table B.8a: Substance-specific input parameters for pesticides

Compound name	Unit	Acephate	Aldicarb	Aldrin	Anilazine	Atrazine	Azinphos-ethyl	Azinphos-methyl	Benomyl	Bentazone	Bifenthrin	Source
CAS nr.	-	30560-19-1	116-06-3	309-00-2	101-05-3	1912-24-9	2642-71-9	86-50-0	17804-35-2	25057-89-0	82657-04-3	
Effects assessment												1-7
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.0 \cdot 10^{-8}$	$3.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-10}$	$1.0 \cdot 10^{-7}$	$3.5 \cdot 10^{-8}$	$2.5 \cdot 10^{-10}$	$5.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-7}$	$2.0 \cdot 10^{-8}$	
Inhalatory Human Limit Value	$kg.m^{-3}$							$2.0 \cdot 10^{-10}$				
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$6.4 \cdot 10^{-6}$	$2.0 \cdot 10^{-8}$	$2.9 \cdot 10^{-8}$	$2.0 \cdot 10^{-7}$	$2.9 \cdot 10^{-6}$	$1.1 \cdot 10^{-8}$	$1.2 \cdot 10^{-8}$	$1.5 \cdot 10^{-7}$	$6.4 \cdot 10^{-5}$	$1.1 \cdot 10^{-9}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	EP[a]	$2.0 \cdot 10^{-9}$	EP[a]	$7.0 \cdot 10^{-9}$	EP[a]	$2.0 \cdot 10^{-8}$	$1.5 \cdot 10^{-9}$	EP[a]	EP[a]	
Physico-chemical properties												2, 8, 9
molecular weight	$g.mol^{-1}$	183.2	190.25	364.93	275.5	215.68	345.4	317.34	290.3	240.3	422.9	
octanol-water partition coefficient	$m^3.m^{-3}$	0.1	13	1000	6300	562	1514	500	200	631	1000000	
melting point	°C	85.4	99.5	104	159.5	174	50	73.5	140	138	58	
vapor pressure (25 °C)	Pa	$2.3 \cdot 10^{-4}$	$4.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	$8.2 \cdot 10^{-7}$	$4.0 \cdot 10^{-5}$	$4.5 \cdot 10^{-4}$	$3.0 \cdot 10^{-5}$	$1.3 \cdot 10^{-8}$	$6.5 \cdot 10^{-4}$	$2.4 \cdot 10^{-5}$	
solubility (25 °C)	$mg.l^{-1}$	818000	6000	$2 \cdot 10^{-2}$	8	30	4.8	30	2	611[b]	0.1	
dissociation constant	-									5		
Partition coefficients												8, 9
organic carbon partition coefficient	$l.kg^{-1}$	2	17	410	1000	155		1300	1900	33	223872	
Degradation rates												2, 9-15
reaction half-life in air	d		$2.4 \cdot 10^{-1}$	$2.3 \cdot 10^{-1}$				$5.4 \cdot 10^{-2}$	$6.7 \cdot 10^{-2}$			
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$5.1 \cdot 10^{-11}$			$1.1 \cdot 10^{-10}$	$1.5 \cdot 10^{-10}$	$1.7 \cdot 10^{-10}$			$1.1 \cdot 10^{-10}$	$3.4 \cdot 10^{-11}$	
hydrolysis in surface water, soil, sediment (PH=6; 12 °C)	d		975	1325	84		21	98	12			
hydrolysis in surface water, soil, sediment (PH=7; 12 °C)	d		1083	1325	57		471	87	12			
hydrolysis in surface water, soil, sediment (PH=8; 12 °C)	d		565	1325	14		167	42	12			
biodegradation in surface water (12 °C)	d	91	148	194	2	780	30	5	30	30	4	
biodegradation in soil (12 °C)	d	4	148	194	2	71	49	79	117	84	382	
aerobic biodegradation in sediment (12 °C)	d	4	148	194	2	71	49	79	117	84	382	
anaerobic biodegradation in sediment (12 °C)	d	15	346	5	7	284	195	314	467	335	1528	
metabolism in plant tissue	d		0.6									
Exposure assessment												9, 16-22
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	1	42	5956		8						
plant conductance	$m.s^{-1}$					$1.18 \cdot 10^{-3}$						
transpiration stream concentration factor	-									0.04[c]		
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$		$9.4 \cdot 10^{-1}$			1.9				0.7[c]		
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$		$3.7 \cdot 10^{-1}$	$2.5 \cdot 10^{-2}$		$2.6 \cdot 10^{-1}$			$3.6 \cdot 10^{-1}$			
biotransfer factor for meat	$d.kg^{-1}$		$9.4 \cdot 10^{-5}$	$8.4 \cdot 10^{-2}$				$7.9 \cdot 10^{-4}$				
biotransfer factor for milk	$d.kg^{-1}$			$1.8 \cdot 10^{-2}$								
bioavailability for inhalation	-			0.3								
bioavailability for oral uptake	-			1								

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [c] assumed default value for dissociating acids at environmental pH of 7, based on Briggs et al. (1987); [1] WHO/FAO (1998); [2] Tomlin (1994); [3] Vermeire et al. (1991); [4] USEPA (1998b); [5] RIZA (1999); [6] Huijbregts (1999); [7] Janssen et al. (1995); [8] Crommentuijn et al. (1997b); [9] Mackay et al. (1997); [10] Howard et al. (1991); [11] RIVM et al. (1998); [12] Jager et al. (1997); [13] Syraceuse Research Corporation (1993); [14] Linders et al. (1994); [15] Howard (1991); [16] Polder et al. (1995); [17] Briggs et al. (1982); [18] Dowdy & McKone (1997); [19] Dowdy et al. (1996); [20] Garten & Trabalka (1983); [21] WHO (1989c); [22] Riederer (1995)

Table B.8b: Substance-specific input parameters for pesticides

Compound name	Unit	Captafol	Captan	Carbaryl	Carbendazim	Carbofuran	Chlordane	Chlorfenvinphos	Chloridazone	Chlorothalonil	Source
CAS nr.	-	2425-06-1		63-25-2	10605-21-7	1563-66-2	57-74-9	470-90-6	1698-60-8	1897-45-6	
Effects assessment											1-7
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$2.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-7}$	$3.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-8}$	$2.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-10}$	$5.0 \cdot 10^{-10}$	$1.6 \cdot 10^{-7}$	$3.0 \cdot 10^{-8}$	
Inhalatory Human Limit Value	$kg.m^{-3}$						$2.0 \cdot 10^{-11}$				
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.8 \cdot 10^{-8}$	$2.2 \cdot 10^{-8}$	$2.3 \cdot 10^{-7}$	$2.0 \cdot 10^{-7}$	$2.0 \cdot 10^{-7}$	$1.5 \cdot 10^{-9}$	$3.3 \cdot 10^{-6}$	$7.3 \cdot 10^{-5}$	$8.8 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$1.5 \cdot 10^{-8}$	$3.0 \cdot 10^{-9}$	$3.7 \cdot 10^{-8}$	$1.8 \cdot 10^{-9}$	$1.2 \cdot 10^{-9}$	$7.0 \cdot 10^{-9}$	$2.2 \cdot 10^{-8}$	$2.3 \cdot 10^{-8}$	EP[a]	
Physico-chemical properties											2, 8, 9
molecular weight	$g.mol^{-1}$	349.1	300.6	201.22	191.19	221.3	409.8	359.56	221.6	265.89	
octanol-water partition coefficient	$m^3.m^{-3}$	3273	200	229	33	209	1000000	6607	14	437	
melting point	°C	160.5	178	142	304.5	151	104	-19	207	250.5	
vapor pressure (25 °C)	Pa	$1.0 \cdot 10^{-10}$	$1.1 \cdot 10^{-5}$	$2.7 \cdot 10^{-5}$	$6.5 \cdot 10^{-8}$	$8.0 \cdot 10^{-5}$	$5.2 \cdot 10^{-4}$	$1.0 \cdot 10^{-4}$	7	$1.3 \cdot 10^{-1}$	
solubility (25 °C)	$mg.l^{-1}$	1.5	5.1	120.0	8.0[b]	351.0	0.1	124.0	360.0	0.6	
dissociation constant	-				4.48						
Partition coefficients											8, 9
organic carbon partition coefficient	$l.kg^{-1}$	2090	200	180	410	43	316228	480	81	1585	
Degradation rates											9-16
reaction half-life in air	d		0.08	0.2		0.2	1.3				
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$8.9 \cdot 10^{-11}$			$2.1 \cdot 10^{-10}$			$5.3 \cdot 10^{-11}$	$4.8 \cdot 10^{-11}$	$6.2 \cdot 10^{-15}$	
hydrolysis in surface water, soil, sediment (PH=6; 12 °C)	d		1	262		110					
hydrolysis in surface water, soil, sediment (PH=7; 12 °C)	d		0.3	26		110					
hydrolysis in surface water, soil, sediment (PH=8; 12 °C)	d		0.3	3		101					
biodegradation in surface water (12 °C)	d	1000	38	12	105	30	1092	36	262	12	
biodegradation in soil (12 °C)	d	1000	38	12	209	26	1092	63	52	37	
aerobic biodegradation in sediment (12 °C)	d	10000	38	12	209	26	1092	63	52	37	
anaerobic biodegradation in sediment (12 °C)	d	40000	153	49	837	46	5	251	209	148	
metabolism in plant tissue	d			2							
Exposure assessment											9, 17-22
bioconcentration factor in fish	$l.kg(wwt)^{-1}$		10	17		118	5594				
transpiration stream concentration factor	-				$8.8 \cdot 10^{-1}$						
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$					1.3					
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$						$1.7 \cdot 10^{-2}$				
biotransfer factor for meat	$d.kg^{-1}$						$1.5 \cdot 10^{-2}$				
biotransfer factor for milk	$d.kg^{-1}$						$4.6 \cdot 10^{-4}$				
bioavailability for oral uptake	-				$8.2 \cdot 10^{-1}$					$3.0 \cdot 10^{-1}$	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [1] FAO/WHO (1998); [2] Tomlin (1994); [3] USEPA (1998b); [4] Janssen et al. (1995); [5] RIZA (1999); [6] Huijbregts (1999); [7] USEPA (1998b); [8] Crommentuijn et al. (1997b); [9] Mackay et al. (1997); [10] Howard et al. (1991); [11] RIVM et al. (1998); [12] Jager et al. (1997); [13] Syraceuse Research Corporation (1993); [14] Linders et al. (1994); [15] Howard (1991); [16] Van Rijn et al. (1995); [17] Sicbaldi et al. (1997); [18] Polder et al. (1995); [19] Dowdy & McKone (1997); [20] Dowdy et al. (1996); [21] WHO (1993a); [22] WHO (1996b)

Table B.8c: Substance-specific input parameters for pesticides

Compound name	Unit	Chlorpropham	Chlorpyriphos	Coumaphos	Cyanazine	Cypermethrin	Cyromazine	2,4-D	DDT	Deltamethrin	Demeton	Source
CAS nr.	-	101-21-3	2921-88-2	56-72-4	21725-46-2	52315-07-8	66215-27-8	94-75-7	50-29-3	52918-63-5	8065-48-3	
Effects assessment												
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$2.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-8}$	$2.5 \cdot 10^{-10}$	$6.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-8}$	$2.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	$2.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	$4.0 \cdot 10^{-11}$	1-6
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$3.8 \cdot 10^{-5}$	$7.4 \cdot 10^{-10}$	$7.4 \cdot 10^{-10}$	$5.0 \cdot 10^{-8}$	$1.3 \cdot 10^{-10}$	$4.5 \cdot 10^{-7}$	$9.9 \cdot 10^{-6}$	$5.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-10}$	$1.4 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	$1.0 \cdot 10^{-9}$	EP[a]	EP[a]	EP[a]	EP[a]	$1.2 \cdot 10^{-8}$	$2.8 \cdot 10^{-8}$	EP[a]	EP[a]	
Physico-chemical properties												
molecular weight	$g.mol^{-1}$	213.65	350.6	362.8	240.7	416.3	166.2	221.04	354.5	505.2	258.34	3, 7, 8
octanol-water partition coefficient	$m^3.m^{-3}$	3240	$8.3 \cdot 10^{4}$	11350	166	$4.0 \cdot 10^{6}$	1	646	$1.6 \cdot 10^{6}$	39810	16	
melting point	°C	40.9	41.5	95	166.75	80.5	221	140.5	108.75	99.5	liquid	
vapor pressure (25 °C)	Pa	$1.0 \cdot 10^{-3}$	$2.3 \cdot 10^{-3}$	$1.8 \cdot 10^{-5}$	$2.1 \cdot 10^{-7}$	$1.9 \cdot 10^{-7}$	$4.5 \cdot 10^{-7}$	$8.0 \cdot 10^{-5}$	$2.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-5}$	$3.5 \cdot 10^{-2}$	
solubility (25 °C)	$mg.l^{-1}$	89	$7.3 \cdot 10^{-1}$	1.6	171	$4.0 \cdot 10^{-3}$	13000	400[b]	$5.5 \cdot 10^{-3}$	$2.0 \cdot 10^{-3}$	60	
dissociation constant	-							3.0				
Partition coefficients												7, 8
organic carbon partition coefficient	$l.kg^{-1}$	347	7590	2089	178	389		46	427000	$4.6 \cdot 10^{5}$	71	
Degradation rates												8-15
reaction half-life in air	d		$2.6 \cdot 10^{-1}$					$4.5 \cdot 10^{-1}$	4.4			
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$4.7 \cdot 10^{-11}$		$1.1 \cdot 10^{-10}$	$1.3 \cdot 10^{-10}$	$3.7 \cdot 10^{-11}$	$1.0 \cdot 10^{-10}$			$3.9 \cdot 10^{-11}$	$1.3 \cdot 10^{-10}$	
hydrolysis in water (PH= 6, 12 °C)	d		209									
hydrolysis in water (PH= 7, 12 °C)	d		92									
hydrolysis in water (PH= 8, 12 °C)	d		3									
biodegradation in water (12 °C)	d	29	37	1000	24	9	269	39	3556	5	30	
hydrolysis in soil (PH=6, 12 °C)	d		2090									
hydrolysis in soil, sediment (PH=7, 12 °C)	d		924									
hydrolysis in sediment (PH=8, 12 °C)	d		26									
biodegradation in soil (12 °C)	d	70	37	1000	24	91	162	39	3556	44	26	
aerobic biodegradation in sediment (12 °C)	d	70	37	10000	49	91	162	39	3556	436	26	
anaerobic biodegradation in sediment (12 °C)	d	279	147	40000	195	362	649	123	70	1744	105	
metabolism in plant tissue	d	1.4						1.8	18.4			
Exposure assessment												8, 15-22
bioconcentration factor in fish	$l.kg(wwt)^{-1}$		752			813		0.1	16549	457		
partitioning coefficient between leaves and air	$m^3.m^{-3}$								$6.74 \cdot 10^{6}$			
plant conductance	$m.s^{-1}$							$4.88 \cdot 10^{-4}$				
transpiration stream concentration factor	-							0.04				
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$							1	4100			
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$				$2.0 \cdot 10^{-1}$				$1.2 \cdot 10^{-2}$			
biotransfer factor for meat	$d.kg^{-1}$		$7.9 \cdot 10^{-4}$	$3.8 \cdot 10^{-6}$				$1.0 \cdot 10^{-5}$	$3.2 \cdot 10^{-2}$			
biotransfer factor for milk	$d.kg^{-1}$		$2.1 \cdot 10^{-5}$	$4.7 \cdot 10^{-6}$				$3.7 \cdot 10^{-6}$	$3.2 \cdot 10^{-3}$			

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [1] Vermeire et al. (1991); [2] FAO/WHO (1998); [3] Environmental Defense Fund (1999); [4] USEPA (1998b); [5] Huijbregts (1999); [6] RIZA (1999); [7] Crommentuijn et al. (1997b); [8] Mackay et al. (1997); [9] Howard et al. (1991); [10] RIVM et al. (1998); [11] Jager et al. (1997); [12] Syraceuse Research Corporation

(1993); [13] Linders et al. (1994); [14] Komoßa et al. (1995); [15] Briggs et al. (1987); [16] Tsuda et al. (1997); [17] Polder et al. (1995); [18] Polder et al. (1998); [19] Devillers et al. (1996); [20] Dowdy & McKone (1997); [21] Dowdy et al. (1996); [22] Riederer (1995)

Table B.8d: Substance-specific input parameters for pesticides

Compound name	Unit	Desmetryn	Diazinon	Dichlorprop	Dichlorvos	Dieldrin	Dimethoate	Dinoseb	Dinoterb	Disulfothon	Diuron	Source
CAS nr.	-	1014-69-3	333-41-5	120-36-5	62-73-7	60-57-1	60-51-5	88-85-7	1420-07-1	298-04-4	330-54-1	
Effects assessment												1-6
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	[a] $1.5 \cdot 10^{-9}$	$2.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-9}$	$4.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-10}$	$2.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-9}$	[b] $3.75 \cdot 10^{-8}$	$3.0 \cdot 10^{-10}$	$2.0 \cdot 10^{-9}$	
Inhalatory Human Limit Value	$kg.m^{-3}$		$9.0 \cdot 10^{-9}$		$5.0 \cdot 10^{-10}$					$2.0 \cdot 10^{-10}$		
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.6 \cdot 10^{-5}$	$3.7 \cdot 10^{-8}$	$4.0 \cdot 10^{-4}$	$7.0 \cdot 10^{-10}$	$2.9 \cdot 10^{-8}$	$2.3 \cdot 10^{-5}$	$2.5 \cdot 10^{-8}$	$3.4 \cdot 10^{-8}$	$2.3 \cdot 10^{-8}$	$4.3 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$2.5 \cdot 10^{-9}$	$1.9 \cdot 10^{-9}$	EP[c]	EP[c]	$3.3 \cdot 10^{-9}$	$1.7 \cdot 10^{-8}$	EP[c]	EP[c]	EP[c]	$2.4 \cdot 10^{-9}$	
Physico-chemical properties												2, 7, 8
molecular weight	$g.mol^{-1}$	213.3	304.36	235.1	220.98	380.93	229.28	240.2	240.2	274.38	233.1	
octanol-water partition coefficient	$m^3.m^{-3}$	240	2000	2690	28	$1.6 \cdot 10^{5}$	6	3630	5495	10500	603	
melting point	°C	85	liquid	116.75	liquid	176.5	52.25	40	126	108	158.5	
vapor pressure (25 °C)	Pa	$1.9 \cdot 10^{-4}$	$8.0 \cdot 10^{-3}$	$4.0 \cdot 10^{-4}$	7.0	$5.0 \cdot 10^{-4}$	$1.0 \cdot 10^{-2}$	$3.2 \cdot 10^{-1}$	$2.8 \cdot 10^{-2}$	$2.0 \cdot 10^{-2}$	$9.2 \cdot 10^{-5}$	
solubility (25 °C)	$mg.l^{-1}$	621	60	350[d]	8000	$1.7 \cdot 10^{-1}$	20000	48.5[d]	4.8[d]	25	40	
dissociation constant	-			3.25				4.5	4.6			
Partition coefficients												7, 8
organic carbon partition coefficient	$l.kg^{-1}$		437	1000	68	12000	58	195		1320	355	
Degradation rates												2, 7, 9-12
reaction half-life in air	d		0.2			1.0	0.1	3.1		0.1		
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$1.4 \cdot 10^{-10}$		$1.1 \cdot 10^{-11}$	$9.2 \cdot 10^{-12}$				$6.2 \cdot 10^{-13}$		$3.4 \cdot 10^{-11}$	
hydrolysis in water, soil, sediment (PH=6, 12 °C)	d		223		5		460			230		
hydrolysis in water, soil sediment (PH=7, 12 °C)	d		316		5		378			230		
hydrolysis in water, soil, sediment (PH=8, 12 °C)	d		317		5		99			230		
biodegradation in water (12 °C)	d	55	47	19	0.8	763	43	127	164	14	47	
biodegradation in soil (12 °C)	d	16	56	21	0.4	763	35	127	17	14	105	
aerobic biodegradation in sediment (12 °C)	d	16	56	21	0.4	763	43	127	17	14	105	
anaerobic biodegradation in sediment (12 °C)	d	63	223	85	2	5	173	14	68	55	420	
metabolism in plant tissue	d						4.2					
Exposure assessment												7, 14-20
bioconcentration factor in fish	$l.kg(wwt)^{-1}$		83		0.6	6166		32	0.8	208	60	
partitioning coefficient between leaves and air	$m^3.m^{-3}$					$1.1 \cdot 10^{6}$						
transpiration stream concentration factor	-			0.04[e]			$4.3 \cdot 10^{-1}$	0.04[e]	0.04[e]		$8.1 \cdot 10^{-1}$	
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$			0.7[e]		43		0.7[e]	0.7[e]		3.1	
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$					$1.0 \cdot 10^{-2}$						
biotransfer factor for meat	$d.kg^{-1}$					$6.8 \cdot 10^{-2}$						
biotransfer factor for milk	$d.kg^{-1}$					$1.2 \cdot 10^{-2}$						

[a] The oral Human Limit Values of Desmetryn is derived by dividing a NOEL for rats (90 days), listed in Tomlin (1994), by a factor 1000 (inter- and intraspecies extrapolation, and extrapolation from subchronic to chronic) (personal assessment); [b] The oral Human Limit Values of Dinoterb is derived by dividing a NOEL for rats (2 years), listed in Tomlin (1994), by a factor 100 (intra- and interspecies extrapolation) (personal assessment); [c] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [d] solubility of the neutral species; [e] assumed default value for dissociating acids at

environmental pH of 7, based on Briggs et al. (1987); [1] FAO/WHO (1998); [2] Tomlin (1994); [3] USEPA (1998b); [4] Environmental Defense Fund (1999); [5] RIZA (1999); [6] Huijbregts (1999); [7] Mackay et al. (1997); [8] Crommentuijn et al. (1997b); [9] Howard et al. (1991); [10] RIVM et al. (1998); [11] Syraceuse Research Corporation (1993) [12] Linders et al. (1994); [13] Komoßa et al. (1995); [14] Sicbaldi et al. (1997); [15] Nendza (1991); [16] Tsuda et al. (1997); [17] Polder et al. (1995); [18] Polder et al. (1998); [19] Dowdy & McKone (1997); [20] Dowdy et al. (1996)

Table B.8e: Substance-specific input parameters for pesticides

Compound name	Unit	DNOC	Endosulfan	Endrin	Ethoprophos	Fenitrothion	Fentin acetate	Fentin chloride	Fentin hydroxide	Fenthion	Folpet	Source
CAS nr.	-	534-52-1	115-29-7	72-20-8	13194-48-4	122-14-5	900-95-8	639-58-7	76-87-9	55-38-9	133-07-3	
Effects assessment												1-5
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.5 \cdot 10^{-10}$	$6.0 \cdot 10^{-9}$	$2.0 \cdot 10^{-10}$	$4.0 \cdot 10^{-10}$	$5.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-10}$	$5.0 \cdot 10^{-10}$	$5.0 \cdot 10^{-10}$	$7.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-7}$	
Inhalatory Human Limit Value	$kg.m^{-3}$	$3.5 \cdot 10^{-10}$										
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$2.1 \cdot 10^{-5}$	$2.0 \cdot 10^{-8}$	$3.0 \cdot 10^{-9}$	$6.3 \cdot 10^{-8}$	$8.7 \cdot 10^{-9}$	$5.0 \cdot 10^{-9}$ (f); $7.8 \cdot 10^{-10}$ (s)	$5.0 \cdot 10^{-9}$ (f); $7.8 \cdot 10^{-10}$ (s)	$5.0 \cdot 10^{-9}$ (f); $7.8 \cdot 10^{-10}$ (s)	$3.1 \cdot 10^{-9}$	$1.2 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$1.9 \cdot 10^{-8}$	$1.5 \cdot 10^{-9}$	EP[a]	EP[a]	EP[a]	$1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	EP[a]	EP[a]	
Physico-chemical properties												6-9
molecular weight	$g.mol^{-1}$	148.1	406.92	380.93	242.3	277.25	409	385.5	367	278.34	296.56	
octanol-water partition coefficient	$m^3.m^{-3}$	138	3980	$1.6 \cdot 10^{5}$	3900	2510	1905	12589	1905	12600	4300	
melting point	°C	86	83.7	209	liquid	liquid	122	166	119	liquid	177	
vapor pressure (25 °C)	Pa	$1.1 \cdot 10^{-2}$	$1.3 \cdot 10^{-3}$	$2.0 \cdot 10^{-5}$	$5.1 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	1	$9.9 \cdot 10^{-6}$	$4.0 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	
solubility (25 °C)	$mg.l^{-1}$	150[b]	0.5	0.23	750	30	9.6	76	1.1	50	1	
dissociation constant	-	4.2										
Partition coefficients												6, 7
organic carbon partition coefficient	$l.kg^{-1}$	219	12300	19500	68	1350	21900	21900	21900	1510	1900	
Degradation rates												7, 9-15
reaction half-life in air	d	77.5	$6.2 \cdot 10^{-1}$	$6.0 \cdot 10^{-2}$								
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$				$6.7 \cdot 10^{-11}$	$6.2 \cdot 10^{-11}$				$7.6 \cdot 10^{-11}$	$1.4 \cdot 10^{-11}$	
hydrolysis in water (PH=6, 12 °C)	d		21			147				351		
hydrolysis in water (PH=7, 12 °C)	d		15			147				349		
hydrolysis in water (PH=8, 12 °C)	d		3.5			145				338		
biodegradation in water (12 °C)	d	21	9	4871	161	22	12.21	12.21	12.21	30	1000	
hydrolysis in soil (PH=6 12 °C)	d		210			147				351		
hydrolysis in soil, sediment (PH=7, 12 °C)	d		150			147				349		
hydrolysis in sediment (PH=8, 12 °C)	d		35			145				338		
biodegradation in soil (12 °C)	d	21	9	4871	56	49	244	244	244	59	1000	
aerobic biodegradation in sediment (12 °C)	d	21	9	4871	56	49	2442	2442	2442	59	1000	
anaerobic biodegradation in sediment (12 °C)	d	8	37	15	223	195	9766	9766	9766	237	4000	
metabolism in plant tissue	d					4						
Exposure assessment												7, 16-22
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	0.2	601	1873		152	1095	1095	1095	759		
transpiration stream concentration factor	-	0.04[c]										
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$	0.7[c]		12								
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$			$1.7 \cdot 10^{-2}$								
biotransfer factor for meat	$d.kg^{-1}$		$7.2 \cdot 10^{-4}$	$1.4 \cdot 10^{-2}$						$2.4 \cdot 10^{-5}$		
biotransfer factor for milk	$d.kg^{-1}$			$2.1 \cdot 10^{-3}$		$7.4 \cdot 10^{-6}$				$6.7 \cdot 10^{-5}$		

bioavailability for oral uptake	-						0.4	0.4	0.4		

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [c] assumed default value for dissociating acids at environmental pH of 7, based on Briggs et al. (1987); f = fresh water; s = salt water; [1] WHO/FAO (1998); [2] FAO/WHO (1999); [3] Environmental Defense Fund (1999); [4] RIZA (1999); [5] Huijbregts (1999); [6] Crommentuijn et al. (1997b); [7] Mackay et al. (1997); [8] Guinée et al. (1996a); [9] Tomlin (1994); [10] Howard et al. (1991); [11] RIVM et al. (1998); [12] Syraceuse Research Corporation (1993); [13] Linders et al. (1994); [14] Jager et al. (1997); [15] Van Rijn et al. (1995); [16] Slooff et al. (1993); [17] Nendza (1991); [18] Tsuda et al. (1997); [19] Polder et al. (1995); [20] Dowdy & McKone (1997); [21] Dowdy et al. (1996); [22] Van de Plassche (1994).

Table B.8f: Substance-specific input parameters for pesticides

Compound name	Unit	Glyphosate	Heptachlor	Heptenophos	Iprodione	Isoproturon	Lindane	Linuron	Malathion	MCPA	Mecoprop	Source
CAS nr.	-	1071-83-6	76-44-8	23560-59-0	36734-19-7	34123-59-6	58-89-9	330-55-2	121-75-5	94-74-6	7085-19-0	
Effects assessment												1-8
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.0 \cdot 10^{-7}$	$1.0 \cdot 10^{-10}$	$5.0 \cdot 10^{-9}$	$6.0 \cdot 10^{-8}$	$6.2 \cdot 10^{-9}$	$1.0 \cdot 10^{-9}$	$2.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-7}$	$1.5 \cdot 10^{-9}$	$1.0 \cdot 10^{-9}$	
Inhalatory Human Limit Value	$kg.m^{-3}$						$2.5 \cdot 10^{-10}$			$7.0 \cdot 10^{-9}$		
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$1.6 \cdot 10^{-6}$	$8.6 \cdot 10^{-9}$	$2.0 \cdot 10^{-8}$	$2.3 \cdot 10^{-6}$	$3.2 \cdot 10^{-6}$	$1.0 \cdot 10^{-6}$	$2.5 \cdot 10^{-7}$	$1.3 \cdot 10^{-8}$	$4.2 \cdot 10^{-5}$	$3.9 \cdot 10^{-6}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP[a]	$2.0 \cdot 10^{-9}$	EP[a]	EP[a]	EP[a]	$2.5 \cdot 10^{-9}$	EP[a]	$5.0 \cdot 10^{-8}$	EP[a]	EP[a]	
Physico-chemical properties												5, 9, 10
molecular weight	$g.mol^{-1}$	169.1	373.4	250.6	330.2	206.3	290.85	249.1	330.36	200.6	214.6	
octanol-water partition coefficient	$m^3.m^{-3}$	$3.1 \cdot 10^{-2}$	$1.9 \cdot 10^{5}$	209	1010	178	5010	1010	631	490	8710	
melting point	°C	200	95.5	liquid	134	155.5	112.5	93.5	2.9	118.5	94.5	
vapor pressure (25 °C)	Pa	$4.0 \cdot 10^{-5}$	$5.3 \cdot 10^{-2}$	$1.7 \cdot 10^{-1}$	$5.0 \cdot 10^{-7}$	$3.3 \cdot 10^{-6}$	$3.7 \cdot 10^{-3}$	$2.3 \cdot 10^{-2}$	$1.0 \cdot 10^{-3}$	$2.0 \cdot 10^{-4}$	$3.1 \cdot 10^{-4}$	
solubility (25 °C)	$mg.l^{-1}$	[b]$1.3 \cdot 10^{5}$	$6.0 \cdot 10^{-2}$	2360	14	55	7.3	75	145	1605[b]	620[b]	
dissociation constant	-	5.7								3.1	3.7	
Partition coefficients												9-11
organic carbon partition coefficient	$l.kg^{-1}$	3630	24000			72	955	603	1170	54	8	
Degradation rates												5, 10, 12-16
reaction half-life in air	d		$2.5 \cdot 10^{-1}$			1.9	2.31	$1.2 \cdot 10^{-1}$	$2.5 \cdot 10^{-1}$	1.3		
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$7.5 \cdot 10^{-11}$		$3.0 \cdot 10^{-11}$	$4.6 \cdot 10^{-11}$						$1.7 \cdot 10^{-11}$	
hydrolysis in water (PH= 6, 12 °C)	d	26	4		11		413					
hydrolysis in water (PH= 7, 12 °C)	d				5		361					
hydrolysis in water (PH= 8, 12 °C)	d				1		159					
biodegradation in water (12 °C)	d	105	54	4	8	74	197	123	26	9	12	
hydrolysis in soil (PH=6, 12 °C)	d	26	41		11		413					
hydrolysis in soil (PH=7, 12 °C)	d				5		361					
biodegradation in soil (12C)	d	105	54	1	72	74	197	123	8	9	12	
hydrolysis in sediment (PH=7, 12 °C)	d	261	405		5		361					
hydrolysis in sediment (PH=8, 12 °C)	d				1		159					
aerobic biodegradation in sediment (12 °C)	d	1046	54	1	72	74	197	123	26	9	12	
anaerobic biodegradation in sediment (12 °C)	d	4186	218	5	286	14	23	493	103	124	49	
metabolism in plant tissue	d	7.9					9.5	8.1	0.6			
Exposure assessment												10, 17-23
bioconcentration factor in fish	$l.kg(wwt)^{-1}$		7427				371		64			
partitioning coefficient between leaves and air	$m^3.m^{-3}$						$3.3 \cdot 10^{5}$					
transpiration stream concentration factor	-	0.04[c]			0.79			0.93		0.04[c]	0.04[c]	
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$	0.7[c]					17			0.7[c]	0.7[c]	
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$		$9.8 \cdot 10^{-3}$				$6.3 \cdot 10^{-2}$					

biotransfer factor for meat	$d.kg^{-1}$		$1.3 \cdot 10^{-2}$				$1.5 \cdot 10^{-2}$		$9.1 \cdot 10^{-6}$		
biotransfer factor for milk	$d.kg^{-1}$		$1.4 \cdot 10^{-3}$				$2.2 \cdot 10^{-3}$		$1.7 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	
bioavailability for oral uptake	-	0.3									

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] solubility of the neutral species; [c] assumed default value for dissociating acids at environmental pH of 7, based on Briggs et al. (1987); [1] FAO/WHO (1998); [2] Janus et al. (1994); [3] RIZA (1999); [4] Huijbregts (1999); [5] Tomlin (1994); [6] Janssen et al. (1998); [7] Environmental Defense Fund (1999); [8] USEPA (1998b); [9] Crommentuijn et al. (1997b); [10] Mackay et al. (1997); [11] Sabljic et al. (1995);); [12] Howard et al. (1991); [13] RIVM et al. (1998); [14] Syraceuse Research Corporation (1993); [15] Linders et al. (1994);[16] Komoßa et al. (1995); [17] Sicbaldi et al. (1997); [18] Polder et al. (1995); [19] Polder et al. (1998); [20] Dowdy & McKone (1997); [21] Dowdy et al. (1996); [22] WHO (1994a); [23] Van de Plassche (1994)

Table B.8g: Substance-specific input parameters for pesticides

Compound name	Unit	Metamitron	Metazachlor	Methabenz-thiazuron	Methomyl	Methyl-bromide	Meto-bromuron	Metolachlor	Mevinphos	Oxamyl	Oxydemethon-methyl	Source
CAS nr.	-	41394-05-2	67129-08-2	18691-97-9	16752-77-5	74-83-9	3060-89-7	51218-45-2	7786-34-7	23135-22-0	301-12-2	
Effects assessment												1-5
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$1.3 \cdot 10^{-7}$	$3.6 \cdot 10^{-8}$	$5.0 \cdot 10^{-8}$	$3.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-6}$	[a] $3.0 \cdot 10^{-8}$	$1.5 \cdot 10^{-7}$	$8.0 \cdot 10^{-10}$	$3.0 \cdot 10^{-8}$	$3.0 \cdot 10^{-10}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$1.0 \cdot 10^{-4}$	$3.4 \cdot 10^{-5}$	$8.4 \cdot 10^{-6}$	$8.0 \cdot 10^{-8}$	$1.1 \cdot 10^{-5}$	$3.6 \cdot 10^{-5}$	$2.0 \cdot 10^{-7}$	$1.6 \cdot 10^{-9}$	$1.8 \cdot 10^{-6}$	$3.5 \cdot 10^{-8}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	EP [b]	EP [b]	EP [b]	EP [b]	EP [b]	EP [b]	$8.3 \cdot 10^{-8}$	EP [b]	EP [b]	EP [b]	
Physico-chemical properties												3, 6-9
molecular weight	$g.mol^{-1}$	202.2	277.8	221.3	162.2	94.94	259.1	283.8	224.1	219.25	246.3	
octanol-water partition coefficient	$m^3.m^{-3}$	5	100	204	4	15	257	1350	3	0.4	0.2	
melting point	°C	166.6	85	120	78.5	-93	95.75	liquid	-56.1	101	-20	
vapor pressure (25 °C)	Pa	$2.0 \cdot 10^{-6}$	$6.9 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$	$6.7 \cdot 10^{-3}$	1700	$4.0 \cdot 10^{-4}$	$4.2 \cdot 10^{-3}$	$1.7 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$5.4 \cdot 10^{-3}$	
solubility (25 °C)	$mg.l^{-1}$	1820	461	63	58000	14000	330	430	$6.0 \cdot 10^{5}$	$2.8 \cdot 10^{5}$	25000	
Partition coefficients												6, 7, 10
Henry's law constant (25 °C)	$Pa.m^3.mol^{-1}$					630						
organic carbon partition coefficient	$l.kg^{-1}$	158	129	631	23		186	214	631	11		
Degradation rates												3, 7, 9, 11-17
reaction half-life in air	d					408			$1.5 \cdot 10^{-1}$			
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$3.7 \cdot 10^{-11}$	$6.7 \cdot 10^{-11}$	$3.2 \cdot 10^{11}$	$1.6 \cdot 10^{-11}$		$3.7 \cdot 10^{-11}$	$7.0 \cdot 10^{-11}$		$2.9 \cdot 10^{-11}$	$1.1 \cdot 10^{-10}$	
hydrolysis in water, soil, sediment (PH=6, 12 °C)	d	54			457	23			209	33	99	
hydrolysis in water, soil sediment (PH=7, 12 °C)	d	54			457	21			61	14	80	
hydrolysis in water, soil, sediment (PH=8, 12 °C)	d	45			457	16			30	2	26	
biodegradation in water (12 °C)	d	33	58	157	400	24	1000	105	9	30	30	
biodegradation in soil (12 °C)	d	52	31	235	52	24	1000	105	4	17	1	
aerobic biodegradation in sediment (12 °C)	d	52	31	235	52	24	1000	105	4	17	1	
anaerobic biodegradation in sediment (12 °C)	d	209	126	942	209	98	4000	419	14	69	4	
metabolism in plant tissue	d				4				1	1.8		
Exposure assessment												7, 9, 17
bioconcentration factor in fish	$l.kg(wwt)^{-1}$							7				
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$									0.9		
bioavailability for oral uptake	-					$5.5 \cdot 10^{-1}$						

[a] The oral Human Limit Values of Metobromuron is derived by dividing a NOEL for dogs (2 years), listed in Tomlin (1994), by a factor 100 (intra- and interspecies extrapolation) (personal assessment); [b] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] FAO/WHO (1998); [2] RIZA (1999); [3] Tomlin (1994); [4] Huijbregts (1999); [5] USEPA (1998b); [6] Crommentuijn et al. (1997b); [7] Mackay et al. (1997); [8] Cambridgesoft Corporation (1998); [9] WHO (1995b); [10] Lide (1993); [11] Howard et al. (1991); [12] RIVM et al. (1998); [13] Syraceuse Research Corporation (1993); [14] Jager et al. (1997); [15] Linders et al. (1994); [16] Van Rijn et al. (1995); [17] Briggs et al. (1982)

Table B.8h: Substance-specific input parameters for pesticides

Compound name	Unit	Parathion-ethyl	Parathion-methyl	Permethrin	Phoxim	Pirimicarb	Propachlor	Propoxur	Pyrazophos	Simazine	Source
CAS nr.	-	56-38-2	298-00-0	52645-53-1	14816-18-3	23103-98-2	1918-16-7	114-26-1	13457-18-6	122-34-9	
Effects assessment											1-4
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$4.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-9}$	$2.0 \cdot 10^{-8}$	$1.3 \cdot 10^{-8}$	$2.0 \cdot 10^{-8}$	$4.0 \cdot 10^{-9}$	$5.0 \cdot 10^{-9}$	
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$1.9 \cdot 10^{-9}$	$1.1 \cdot 10^{-8}$	$3.0 \cdot 10^{-10}$	$8.2 \cdot 10^{-8}$	$8.2 \cdot 10^{-8}$	$1.3 \cdot 10^{-6}$	$1.0 \cdot 10^{-8}$	$4.0 \cdot 10^{-8}$	$1.4 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$1.0 \cdot 10^{-9}$	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	EP[a]	$1.4 \cdot 10^{-9}$	
Physico-chemical properties											5-7
molecular weight	$g.mol^{-1}$	291.27	263.5	391.3	298.3	238.3	211.7	209.24	373.4	201.7	
octanol-water partition coefficient	$m^3.m^{-3}$	6310	1010	$1.3 \cdot 10^{6}$	2400	50	151	32	6300	151	
melting point	°C	6	37.5	36.4	6.1	90.5	71.4	91.5	51.5	226	
vapor pressure (25 °C)	Pa	$6.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$1.7 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	$9.7 \cdot 10^{-4}$	$3.0 \cdot 10^{-2}$	$1.7 \cdot 10^{-5}$	$4.6 \cdot 10^{-5}$	$8.5 \cdot 10^{-6}$	
solubility (25 °C)	$mg.l^{-1}$	12.4	25	$1.0 \cdot 10^{-2}$	$1.6 \cdot 10^{-3}$	3210	600	1800	4.2	5	
Partition coefficients											5, 7
organic carbon partition coefficient	$l.kg^{-1}$	10500	1480	24500		417	79	22		110	
Degradation rates											5, 6, 8-12
reaction half-life in air	d		$2.6 \cdot 10^{-1}$					$1.8 \cdot 10^{-1}$			
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$	$9.0 \cdot 10^{-11}$		$3.9 \cdot 10^{-11}$	$9.8 \cdot 10^{-11}$	$2.3 \cdot 10^{-10}$	$2.2 \cdot 10^{-11}$		$1.1 \cdot 10^{-10}$	$1.4 \cdot 10^{-10}$	
hydrolysis in water (PH=6, 12 °C)	d	112	94		12			2964			
hydrolysis in water (PH=7, 12 °C)	d	328	94		13			372			
hydrolysis in water (PH=8, 12 °C)	d	183	89		10			30			
biodegradation in water (12 °C)	d	37	57	35	1000	30	14	24	17	37	
hydrolysis in soil (PH=6, 12 °C)	d	1120	94		12			2964			
hydrolysis in soil (PH=7, 12 °C)	d	3280	94		13			372			
biodegradation in soil (12C)	d	37	105	35	1000	188	11	24	68	105	
hydrolysis in sediment (PH=7, 12 °C)	d	3280	936		13			372			
hydrolysis in sediment (PH=8, 12 °C)	d	1830	889		10			30			
aerobic biodegradation in sediment (12 °C)	d	37	57	35	1000	188	11	24	68	105	
anaerobic biodegradation in sediment (12 °C)	d	147	5	138	4000	753	43	98	272	420	
metabolism in plant tissue	d	0.7									
photodegradation upon plant tissue	d	20.3				1.6					
Exposure assessment											5, 13-19
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	159	302	2522							
transpiration stream concentration factor	-									0.9	
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$									4.5	
bioconcentration factor from soil to leafs	$kg(wwt).kg(wwt)^{-1}$									0.2	

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [1] FAO/WHO (1998); [2] RIZA (1999); [3] Huijbregts (1999); [4] USEPA (1998b); [5] Mackay et al. (1997); [6] Tomlin (1994); [7] Crommentuijn et al. (1997b); [8] Howard et al. (1991); [9] RIVM et al. (1998); [10] Syracuse Research Corporation (1993); [11] Jager et al. (1997); [12] Linders et al. (1994); [13] Schwack et al. (1994); [14] Schynowski & Schwack (1996); [15] Cabras et al. (1990); [16] Komoßa et al. (1995); [17] Sicbaldi et al. (1997); [18] Polder et al. (1995); [19] Dowdy & McKone (1997)

Table B.8i: Substance-specific input parameters for pesticides

Compound name	Unit	2,4,5-T	Thiram	Tolclophos-methyl	Tri-allaat	Triazophos	Tributyltin-oxide	Trichlorfon	Trifluralin	Zineb	Source
CAS nr.	-	93-76-5	137-26-8	57018-04-9	2303-17-5	24017-47-8	56-35-9	52-68-6	1582-09-8	12122-67-7	
Effects assessment											1-6
Oral Human Limit Value	$kg.kg(bw)^{-1}.d^{-1}$	$3.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$	$7.0 \cdot 10^{-8}$	$1.3 \cdot 10^{-8}$	$1.0 \cdot 10^{-9}$	$3.0 \cdot 10^{-10}$	$1.0 \cdot 10^{-8}$	$7.5 \cdot 10^{-9}$	$3.0 \cdot 10^{-8}$	
Inhalatory Human Limit Value	$kg.m^{-3}$						$2.0 \cdot 10^{-11}$				
Aquatic Predicted No Effect Concentration	$kg.m^{-3}$	$1.6 \cdot 10^{-4}$	$3.2 \cdot 10^{-8}$	$7.9 \cdot 10^{-7}$	$8.0 \cdot 10^{-8}$	$3.2 \cdot 10^{-8}$	$1.4 \cdot 10^{-8}$ (f); $1.0 \cdot 10^{-9}$ (s)	$1.0 \cdot 10^{-9}$	$2.6 \cdot 10^{-8}$	$2.0 \cdot 10^{-7}$	
Terrestrial Predicted No Effect Concentration	$kg.kg(dwt)^{-1}$	$1.5 \cdot 10^{-8}$	EP[a]	EP[a]	$4.4 \cdot 10^{-9}$	EP[a]	EP[a,]	EP[a]	$1.4 \cdot 10^{-9}$	EP[a]	
Physico-chemical properties											7-11
molecular weight	$g.mol^{-1}$	255.5	240.4	301.1	304.7	313.3	596	257.45	335.5	275.8	
octanol-water partition coefficient	$m^3.m^{-3}$	1350	54	36000	19500	2794	6310	3	$2.2 \cdot 10^{5}$	20	
melting point	°C	153	145	79	29.5	3.2	-45	83.5	48.75	157	
vapor pressure (25 °C)	Pa	$5.0 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	$5.7 \cdot 10^{-2}$	$1.5 \cdot 10^{-2}$	$2.8 \cdot 10^{-4}$	$1.4 \cdot 10^{-3}$	$1.0 \cdot 10^{-3}$	$2.6 \cdot 10^{-2}$	$1.3 \cdot 10^{-5}$	
solubility (25 °C)	$mg.l^{-1}$	220[c]	30	0.3	4	37.1	71.2	154000	0.5	10	
dissociation constant	-	2.9									
Partition coefficients											7, 8
organic carbon partition coefficient	$l.kg^{-1}$	98	490	2000	1380	355	12600	38	8510	400	
Degradation rates											8-10, 12-19
reaction half-life in air	d	3.1	26.6					2.5			
hydroxyl radical reaction in air	$cm^3.molec^{-1}.s^{-1}$			$6.3 \cdot 10^{-11}$	$3.2 \cdot 10^{-11}$	$1.1 \cdot 10^{-10}$			$8.4 \cdot 10^{-11}$		
hydrolysis in water, soil, sediment (PH=6, 12 °C)	d		56					8			
hydrolysis in water, soil sediment (PH=7, 12 °C)	d		31					4			
hydrolysis in water, soil, sediment (PH=8, 12 °C)	d		5					2			
biodegradation in water (12 °C)	d	25	1000	53	105	61	224	12	105	63	
biodegradation in soil (12 °C)	d	25	1000	115	12	113	244	12	105	49	
aerobic biodegradation in sediment (12 °C)	d	25	1000	115	12	113	244	12	105	49	
anaerobic biodegradation in sediment (12 °C)	d	124	4000	460	47	453	976	47	49	195	
metabolism in plant tissue	d	7.8									
Exposure assessment											8, 10, 20-24
bioconcentration factor in fish	$l.kg(wwt)^{-1}$	43		579			510		3467		
partitioning coefficient between leaves and air	$m^3.m^{-3}$								$1.0 \cdot 10^{5}$		
plant conductance	$m.s^{-1}$	$6.39 \cdot 10^{-4}$									
transpiration stream concentration factor	-	0.04[d]									
bioconcentration factor from porewater to roots	$l.kg(wwt)^{-1}$	0.7[d]									
biotransfer factor for meat	$d.kg^{-1}$	$2.0 \cdot 10^{-5}$							$9.4 \cdot 10^{-7}$		
biotransfer factor for milk	$d.kg^{-1}$	$2.0 \cdot 10^{-5}$									
bioavailability for oral uptake	-						$3.5 \cdot 10^{-1}$				

[a] EP = $PNEC_{soil}$ derived by Equilibrium Partitioning; [b] The fresh water PNEC is used in the derivation of the soil PNEC; [c] solubility of the neutral species; [d] default value for dissociating acids at environmental pH of 7, based on Briggs et al. (1987); f = fresh water; s = salt water; [1] FAO/WHO (1998); [2] RIZA (1999); [3] USEPA (1998b); [4] Janssen et al. (1995); [5] Huijbregts (1999); [6]

Environmental Defense Fund (1999); [7] Crommentuijn et al. (1997b); [8] Mackay et al. (1997); [9] Tomlin (1994); [10] Slooff et al. (1993); [11] Guinée et al. (1996a); [12] Howard et al. (1991); [13] RIVM et al. (1998); [14] Howard (1991); [15] Syraceuse Research Corporation (1993); [16] Jager et al. (1997); [17] Linders et al. (1994); [18] Van Rijn et al. (1995); [19] Komoßa et al. (1995); [20] Paterson et al. (1991); [21] Tsuda et al. (1997); [22] Dowdy et al. (1996); [23] Garten & Trabalka (1983); [24] Riederer (1995)