

Appendix A
Table 5 - Physical and Toxicological Properties
A. Organic Regulated Substances

Regulated Substance	CAS	RfDo (mg/kg-d)	CSFo (mg/kg-d)-1	RfDi (mg/kg-d)	CSFi (mg/kg-d)-1	Koc	VOC?	Aqueous Sol (mg/L)	Aqueous Sol Reference ¹	TF Vol from Surface Soil	TF Vol from SubSurface Soil	Organic Liquid	Boiling Point (degrees C)	Degradation Coefficient (K/yr ¹)
ACENAPHTHENE	83-32-9	0.06 I		0.06 Ir		4900		3.8	1.5,6				279	1.24
ACENAPHTHYLENE	208-96-8	0.06 S		0.06 S		4500		16.1	5,6,7				280	2.11
ACEPHATE	30560-19-1	0.004	0.0087			3		818000	6					
ACETALDEHYDE	75-07-0		0.0077 Ir	0.0026 I	0.0077 I	4.1	X	1000000	1	13100	15100	X	20	
ACETONE	67-64-1	0.1 I		8.86 D		0.31	X	1000000	1	13100	15000	X	56	18.07
ACETONITRILE	75-05-8			0.017 I		0.5	X	1000000	1	13100	15000	X	82	4.50
ACETOPHENONE	98-86-2	0.1 I		0.1 Ir		170		5500	1			X	203	
ACETYLAMINOFLUORENE, 2- (2AAF)	53-96-3		3.8 C		3.8 C	1600		10.13	7				303	0.69
ACROLEIN	107-02-8	0.02 H				0.56	X	208000	1,2,4	13100	15100	X	53	4.50
ACRYLAMIDE	79-06-1	0.0002 I	4.5 Ir	0.0002 Ir	4.55 I	25	X	2151000	4			X	192.6	
ACRYLIC ACID	79-10-7	0.5 I		0.000286 I		29	X	1000000	2	13000	14900	X	141	1.39
ACRYLONITRILE	107-13-1	0.001 H	0.54 I	0.000571 I	0.238 I	11	X	73500	1	13100	15100	X	77	5.50
ALACHLOR	15972-60-8	0.01 I	0.08 H	0.01	0.08 Hr	110		140	2				100	
ALDICARB	116-06-3	0.001 I		0.001 Ir		22		6000	2				287	0.40
ALDRIN	309-00-2	0.00003 I	17 I	0.00003 Ir	17.15 I	48000		0.02	4,5,6				145	0.22
ALLYL ALCOHOL	107-18-6	0.005 I		0.005 Ir		3.2	X	1000000	2	13100	15000	X	97	18.07
AMINOBIIPHENYL, 4-	92-67-1		21 C		21 C	110		1200	5				302	18.07
AMITROLE	61-82-5		0.94 C		0.945 C	120		280000	4				200	0.69
AMMONIA	7664-41-7	0.97 H		0.0286 I		3	X	310000	2,5,7	13100	15000	X	-33.3	
AMMONIUM SULFAMATE	7773-06-0	0.2 I		0.2		3		2160000	10				200	
ANILINE	62-53-3	0.007 N	0.0057 I	0.000286 I	0.0056 C	190	X	33800	1	13000	14900	X	184	
ANTHRACENE	120-12-7	0.3 I		0.3		21000		0.066	1,5,6,7,8,9				340	0.28
ATRAZINE	1912-24-9	0.035 I	0.222 H	0.035 I	0.222 Hr	130		70	2,4,5				200	
BAYGON (PROPOXUR)	114-26-1	0.004 I		0.004		31		2000	2,4,5				decomp.	4.50
BENOMYL	17804-35-2	0.05 I				1,900		2	5					
BENTAZON	25057-89-0	0.03 I				13		500	2					
BENZENE	71-43-2	0.003 N	0.029 I	0.0017 N	0.027 I	58	X	1780.5	1,2,3,4	13100	15000	X	81	0.35
BENZIDINE	92-87-5	0.003 I	230 I	0.003	230 I	530,000		520	1,2,4				400	15.81
BENZO[A]ANTHRACENE	56-55-3		0.73 N		0.31 T	350000		0.011	1,5,6				438	0.19
BENZO[A]PYRENE	50-32-8		7.3 I		3.1 N	910000		0.0038	1,5,6				495	0.24
BENZO[B]FLUORANTHENE	205-99-2		0.73 N		0.31 T	550000		0.0012	5,6,7				357	0.21
BENZO[G]HIPPERYLENE	191-24-2	0.06 S		0.06 S		2800000		0.00026	1,5,6				500	0.19
BENZO[K]FLUORANTHENE	207-08-9		0.073 N	0.06	0.031 T	4400000		0.00055	5,6,7				480	0.06
BENZOIC ACID	65-85-0	4 I		4 Ir		32		2700	2,3,4,5				249	
BENZOTRICHLORIDE	98-07-7		13 I			920		53	1,5,13			X	220.8	121413.60
BENZYL ALCOHOL	100-51-6	0.3 H		0.3 Hr		100		40000	1,2,3			X	205	
BENZYL CHLORIDE	100-44-7		0.17 I		0.1715 C	190	X	493	1	13000	15000	X	179	20.90
BHC, ALPHA	319-84-6	0.008 D	6.3 I	0.0006 S	6.3 I	1800		1.7	4,5,6,7				288	0.94
BHC, BETA-	319-85-7	0.0006 D	1.8 I	0.0006 Dr	1.855 I	2300		0.1	6				60	1.02
BHC, DELTA-	319-86-8	0.0006 S		0.0006 S		1900		8	6				60	1.26
BHC, GAMMA (LINDANE)	58-89-9	0.0003 I	1.3 H	0.0003 Ir	1.085 C	1400		7.3	4,5,6				323	1.05
BIPHENYL, 1,1-	92-52-4	0.05 I		0.05 Ir		1,700		7.2	1				255	18.07
BIS(2-CHLOROETHYL)ETHER	111-44-4		1.1 I		1.155 I	76	X	10200	1,4,5	13000	14900	X	179	0.69
BIS(2-CHLORO-ISOPROPYL)ETHER	108-60-1	0.04 I	0.07 H	0.04 Ir	0.035 H	62	X	1700	5	13000	14900	X	189	0.69
BIS(CHLOROMETHYL)ETHER	542-88-1		220 I		217 I	16	X	22000	6	13100	15100	X	105	57270.57
BIS(2-ETHYLHEXYL) PHTHALATE	117-81-7	0.02 I	0.014 I	0.02 Ir	0.014 N	87000		0.285	4,5,6			X	384	0.65
BISPHENOL A	80-05-7	0.05 I				1,500		120	4				220	0.69
BROMACIL	314-40-9	0.1 M				58		815	2					
BROMOCHLOROMETHANE	74-97-5	0.01 M				27	X	16700	4	13100	15000	X	68	
BROMODICHLOROMETHANE	75-27-4	0.02 I	0.062 I	0.02 Ir	0.1295 C	93	X	4500	6	13100	15000	X	87	
BROMOMETHANE	74-83-9	0.0014 I		0.0014 I		170	X	17500	2	13100	15000	X	4	6.66
BROMOXYNIL	1689-84-5	0.02 I				300		130	2					
BROMOXYNIL OCTANOATE	1689-99-2	0.02 I				18,000		0.08	12					5.75
BUTADIENE, 1,3-	106-99-0		3.4 C		0.98 I	120		735	1				-4.5	4.50
BUTYL ALCOHOL, N-	71-36-3	0.1 I		0.1 Ir		3.2	X	74000	1	13000	14900	X	118	4.68
BUTYLATE	2008-41-5	0.05 I				540	X	45	2	13200	15200	X	138	
BUTYLBENZENE, N-	104-51-8	0.04 N				2,500	X	15	1,6,7	13100	15100	X	183.1	
BUTYLBENZENE, SEC-	135-98-8	0.04 N				890	X	17	1,6,7	13100	15000	X	173.5	
BUTYLBENZENE, TERT-	98-06-6	0.04 N				680	X	30	1,6,7	13100	15000	X	169	
BUTYLBENZYL PHTHALATE	85-68-7	0.2 I		0.2 Ir		34000		2.69	4,5,6			X	370	1.39
CAPTAN	133-06-2	0.13 I	0.0035 H	0.13 Ir	0.00231 C	200		0.5	4				259	589.39
CARBARYL	63-25-2	0.1 I		0.1 Ir		190		120	2,4,5				315	4.22
CARBAZOLE	86-74-8		0.02 H			2,500		1.2	1,5,6				355	
CARBOFURAN	1563-66-2	0.005 I		0.005 Ir		43		700	2				200	
CARBON DISULFIDE	75-15-0	0.1 I		0.2 I		300	X	2100	1,2,3	13100	15100	X	46	
CARBON TETRACHLORIDE	56-23-5	0.0007 I	0.13 I	0.00057 N	0.0525 I	160	X	795	1,2,3	13100	15000	X	77	0.07
CARBOXIN	5234-68-4	0.1 I				260		170	5,6,8					
CHLORAMBEN	133-90-4	0.015 I		0.015 Ir		20		700	2				210	

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CHLORDANE	57-74-9	0.0005 I	0.35 I	0.0002 I	0.35 I	98000		0.056	4.5,7				175	0.091
CHLORO-1,1-DIFLUOROETHANE, 1-	75-68-3			14.3 I		22		1400	4				-9.2	
CHLORO-1-PROPENE, 3- (ALLYL CHLORIDE)	107-05-1	0.000286 Ir	0.021 C	0.000286 I	0.021 C	48	X	3300	1,3,5,7,10	13100	15000	X	45	18.07
CHLOROACETOPHENONE, 2-	532-27-4	0.00000857 Ir		0.00000857 I		76		1100	3				247	4.50
CHLOROANILINE, P-	106-47-8	0.004 I		0.004 Ir		460		3900	1				232	
CHLOROBENZENE	108-90-7	0.02 I		0.00571 H		200	X	490	3			X	132	0.84
CHLOROBENZILATE	510-15-6	0.02 I	0.27 H	0.02 Ir	0.273 H	2600		13	4			X	415	3.60
CHLOROBUTANE, 1-	109-69-3	0.4 H				580	X	680	1,2,3,4	13200	15000	X	78.5	
CHLORODIBROMOMETHANE	124-48-1	0.02 I	0.084 I	0.02 Ir	0.0945 C	83	X	4200	4,6,7,9	13100	15100	X	116	1.39
CHLORODIFLUOROMETHANE	75-45-6			14 I		59	X	2899	4	13200	15000	X	-40.8	
CHLOROETHANE	75-00-3	0.4 Ir	0.0029 N	2.86 I		42	X	5700	1	13100	15000	X	12	4.50
CHLOROFORM	67-66-3	0.01 I	0.0061 I	0.00009 N	0.0805 I	56	X	8000	1,2,3	13100	15000	X	61	0.01
CHLORONAPHTHALENE, 2-	91-58-7	0.08 I		0.08 Ir		8500		11.7	1				256	
CHLORONITROBENZENE, P-	100-00-5		0.018 H			480		220	1				242	
CHLOROPHENOL, 2-	95-57-8	0.005 I		0.005 Ir		400	X	24000	1,3,4	12900	14900	X	175	
CHLOROPRENE	126-99-8	0.02 H		0.002 H		50	X	1736	9	13100	15000	X	59	0.69
CHLOROPROPANE, 2-	75-29-6			0.0286 H		260	X	3100	1,3,5	13200	15000	X	47.2	
CHLOROTHALONIL	1897-45-6	0.015 I	0.011 H		0.0031 C	980		0.6	2				350	
CHLOROTOLUENE, O-	95-49-8	0.02 I				760	X	422	14,15	13100	15000	X	158.97	
CHLORPYRIFOS	2921-88-2	0.003 I		0.003 Ir		4600		1.12	2,4,6,7				200	
CHLORSULFURON	64902-72-3	0.05 I				11		192	2,5,6,8,9				152	
CHLORTHAL-DIMETHYL (DACTHAL) (DCPA)	1861-32-1	0.01 I				6,500		0.5	2,5,7				360	1.37
CHRYSENE	218-01-9		0.0073 N		0.0031 T	490000		0.0019	1				448	0.126
CRESOL(S)	1319-77-3	0.005 S				25	X	20000	2	13000	14900	X	139	5.16
CRESOL, O- (METHYLPHENOL, 2-)	95-48-7	0.05 I				97	X	2500	3,5,6	12900	14800	X	191	18.07
CRESOL, M (METHYLPHENOL, 3-)	108-39-4	0.05 I				35		2500	2			X	202	5.16
CRESOL, P (METHYLPHENOL, 4-)	106-44-5	0.005 H				49		22000	6				202	9.03
CRESOL, P-CHLORO-M-	59-50-7	0.005 S				780		3846	2				235	
CROTONALDEHYDE	4170-30-3		1.9 S		1.9 Sr	5.6	X	180000	3			X	104	18.07
CROTONALDEHYDE, TRANS-	123-73-9		1.9 H		1.9 Hr	6.1	X	156000	1	13100	15100	X	104	18.07
CUMENE	98-82-8	0.1 I		0.4 I		2800	X	50	1,5,6	13100	15100	X	152	15.81
CYCLOHEXANONE	108-94-1	5 I		5 Ir		66	X	36500	1,2,4,5	13000	14900	X	157	
CYFLUTHRIN	68359-37-5	0.025 I				130,000	X	0.001	2	13000	15000	X		
CYROMAZINE	66215-27-8	0.0075 I				1,200		11000	12				222	
DDD, 4,4'-	72-54-8		0.24 I		0.2415 C	44000		0.16	5,6,7				193	0.02
DDE, 4,4'-	72-55-9		0.34 I		0.34 C	87000		0.04	5				348	0.02
DDT, 4,4'-	50-29-3	0.0005 I	0.34 I	0.0005 Ir	0.34 I	240000		0.0055	5,6,7				260	0.02
DI(2-ETHYLHEXYL)ADIPATE	103-23-1	0.6 I	0.0012 I			47,000,000		200	5	13000	14900	X	214	4.50
DIALLATE	2303-18-4		0.061 H		0.061 Hr	190	X	40	2,4,6,8	12900	14900	X	150	1.39
DIAMINOTOLUENE, 2,4-	95-80-7		3.2 H		4 C	36		7470	4				292	0.69
DIAZINON	333-41-5	0.0009 H		0.0009 Hr		500		50	2,4,6,8				306	
DIBENZO[A,H]ANTHRACENE	53-70-3		7.3 N		3.1 T	1800000		0.0006	1,5,6				524	0.13
DIBROMO-3-CHLOROPROPANE, 1,2-	96-12-8	0.0000571 Ir	1.4 H	0.0000571 I	0.00242 H	140	X	1000	4	13000	15000	X	196	0.69
DIBROMOBENZENE, 1,4-	106-37-6	0.01 I				1,600		20	1				220.4	
DIBROMOETHANE, 1,2- (ETHYLENE DIBROMIDE)	106-93-4	0.0000571 Hr	85 I	0.0000571 H	0.77 I	54	X	4150	1,2,3,5	13100	15100	X	131	2.11
DIBROMOMETHANE	74-95-3	0.01 H		0.01 Hr		110	X	11400	1	13100	15100	X	96	4.50
DIBUTYL PHTHALATE, N-	84-74-2	0.1 I		0.1 Ir		1600		400	1,2,3			X	340	11.00
DICHLORO-2-BUTENE, 1,4-	764-41-0				9.3 H	180		850	9				156	
DICHLOROBENZENE, 1,2-	95-50-1	0.09 I		0.0571 H		350	X	147	1,4,5,6,7	13100	15100	X	180	0.69
DICHLOROBENZENE, 1,3-	541-73-1	0.03 N				360	X	106	1	13100	15100	X	173	0.69
DICHLOROBENZENE, P-	106-46-7	0.03 N	0.024 H	0.229 I	0.022 N	510		82.9	1				174	0.69
DICHLOROBENZIDINE, 3,3'-	91-94-1		0.45 I		1.19 C	22000		3.11	4,5,6				368	0.69
DICHLORODIFLUOROMETHANE (FREON 12)	75-71-8	0.2 I		0.0571 H		360	X	280	1	13200	15000	X	-30	0.69
DICHLOROETHANE, 1,1-	75-34-3	0.1 H	0.0057 C	0.143 H	0.0056 C	52	X	5000	2	13100	15000	X	57	0.16
DICHLOROETHANE, 1,2-	107-06-2	0.03 N	0.091 I	0.23 D	0.091 I	38	X	8412	1,2,3,4	13100	15000	X	83	0.69
DICHLOROETHYLENE, 1,1-	75-35-4	0.009 I	0.6 I	0.009 Ir	0.175 I	65	X	2500	1,4,5	13100	15000	X	32	0.19
DICHLOROETHYLENE, CIS-1,2-	156-59-2	0.01 I		0.01 Ir		49	X	3500	1	13100	15000	X	60	0.01
DICHLOROETHYLENE, TRANS-1,2-	156-60-5	0.02 I		0.02 Ir		47	X	6300	1	13100	15000	X	48	0.01
DICHLOROMETHANE (METHYLENE CHLORIDE)	75-09-2	0.06 I	0.0075 I	0.857 H	0.00165 I	16	X	20000	1,2,3	13100	15000	X	40	4.50
DICHLOROPHENOL, 2,4-	120-83-2	0.003 I		0.003 Ir		160		4500	1				210	5.88
DICHLOROPHOXYACETIC ACID, 2,4- (2,4-D)	94-75-7	0.01 I		0.01 Ir		59		677	4,5,6,7,10				215	1.39
DICHLOROPROPANE, 1,2-	78-87-5	0.09 D	0.068 H	0.0011 I	0.036 C	47	X	2700	1,3,4	13100	15000	X	96	0.10
DICHLOROPROPENE, 1,3-	542-75-6	0.03 I	0.1 I	0.0057 I	0.014 I	27	X	2700	6	13100	15000	X	108	22.38
DICHLOROPROPIONIC ACID (DALAPON), 2,2-	75-99-0	0.03 I		0.03 Ir		62	X	500000	5	13000	14900	X	190	2.11
DICHLORVOS	62-73-7	0.0005 I	0.29 I	0.000143 I	0.291 C	50		10000	2,4,5				140	
DICYCLOPENTADIENE	77-73-6	0.03 H		0.0000571 H		810	X	40	5			X	167	
DIELDRIN	60-57-1	0.00005 I	16 I	0.00005 Ir	16.1 I	11000		0.17	4,5,6			X	385	0.12
DIETHYL PHTHALATE	84-66-2	0.8 I		0.8 Ir		81		1080	4,5,6			X	298	2.25

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DIFLUBENZURON	35367-38-5	0.02 I				1,000		0.2	2				201	
DIMETHOATE	60-51-5	0.0002 I		0.0002 Ir		110		25000	4				200	2.26
DIMETHOXYBENZIDINE, 3,3-	119-90-4		0.014 H			1,300		60	9				331	0.69
DIMETHYLAMINOAZOBENZENE, P-	60-11-7		4.6 C		4.55 C	1000		13.6	7				200	4.50
DIMETHYLANILINE, N,N-	121-69-7	0.002 I				180	X	1200	5,6,7,9	13000	14900	X	192	0.69
DIMETHYLBENZIDINE, 3,3-	119-93-7		9.2 H		9.2 Hr	22,000		1300	10			X	300	18.07
DIMETHYLPHENOL, 2,4-	105-67-9	0.02 I		0.02 Ir		130		7869	1,4,6,7			X	211	18.07
DINITROBENZENE, 1,3-	99-65-0	0.0001 I		0.0001 Ir		150		523	3,5,6,7				300	0.69
DINITROPHENOL, 2,4-	51-28-5	0.002 I		0.002 Ir		0.79		5600	2,4,5,6,7					0.48
DINITROTOLUENE, 2,4-	121-14-2	0.002 I	0.31 C	0.002 Ir	0.31 C	51		270	4,5,6				300	0.69
DINITROTOLUENE, 2,6- (2,6-DNT)	606-20-2	0.001 H		0.001 Hr		74		200	6				300	0.69
DINOSEB	88-85-7	0.001 I		0.001 Ir		120		50	5				223	1.03
DIOXANE, 1,4-	123-91-1		0.011 I			0.027 C	X	1000000	5	13000	14900	X	101	0.69
DIPHENAMID	957-51-7	0.03 I				200		280	5				210	
DIPHENYLAMINE	122-39-4	0.025 I		0.025 Ir		190		300	3				302	4.50
DIPHENYLHYDRAZINE, 1,2-	122-66-7		0.8 I		0.77 I	660		0.252	6				309	0.69
DIQUAT	85-00-7	0.0022 I		0.0022 Ir		2.6		700000	5				355	
DISULFOTON	298-04-4	0.00004 I		0.00004 Ir		1000	X	25	4,5,6	13400	15400	X	133	6.02
DIURON	330-54-1	0.002 I		0.002 Ir		300		42	2,4,5					
ENDOSULFAN	115-29-7	0.006 I		0.006 Ir		2,000		0.48	4				106	2.78
ENDOSULFAN I (ALPHA)	959-98-8	0.006 S		0.006 Sr		2000		0.5	6				200	
ENDOSULFAN II (BETA)	33213-65-9	0.006 S		0.006 Sr		2300		0.45	6				390	
ENDOSULFAN SULFATE	1031-07-8	0.006 S		0.006 Sr		2300		0.117	7,9				200	
ENDOTHALL	145-73-3	0.02 I		0.02 Ir		120		100000	2				200	
ENDRIN	72-20-8	0.0003 I		0.0003 Ir		11000		0.23	4,6,7,9				245	
EPICHLOROHYDRIN	106-89-8	0.002 H	0.0099 I	0.000286 I	0.0042 I	35	X	65800	1,3,4	13000	14900	X	116	4.50
ETHEPHON	16672-87-0	0.005 I				2		1240000	12				201	
ETHION	563-12-2	0.0005 I		0.0005 Ir		8700		0.85	4,6,9,10			X	200	
ETHOXYETHANOL, 2- (EGEE)	110-80-5	0.4 H		0.057 I		12	X	1000000	2	13200	15000	X	136	4.50
ETHYL ACETATE	141-78-6	0.9 I		0.9 Ir		59	X	80800	1,2,3,4,5,6	13100	15000	X	77	18.07
ETHYL ACRYLATE	140-88-5		0.048 H		0.048 Hr	110	X	15000	1,2,6	13100	15100	X	100	18.07
ETHYL BENZENE	100-41-4	0.1 I		0.286 I		220	X	161	1,3,4	13100	15000	X	136	1.11
ETHYL DIPROPYLTHIOCARBAMATE, S- (EPTC)	759-94-4	0.025 I				240	X	365	2	12900	14900	X	127	
ETHYL ETHER	60-29-7	0.2 I		0.2 Ir		68	X	60400	1	13100	15100	X	35	
ETHYL METHACRYLATE	97-63-2	0.09 H		0.09 Hr		22		4635.5	9,10				117	
ETHYLENE GLYCOL	107-21-1	2 I		2 Ir		4.4	X	1000000	2	13100	15100	X	198	10.54
ETHYLENE THIOUREA (ETU)	96-45-7	0.00008 I	0.11 H	0.00008 Ir	0.045 C	0.23		20000	2				450	
ETHYL-P-NITROPHENYL PHENYLPHOSPHOROTHIOATE	2104-64-5	0.00001 I				1,200		3.1	4				215	
FENAMIPHOS	22224-92-6	0.00025 I		0.00025 Ir		300		329	2				200	
FENVALERATE (PYDRIN)	51630-58-1	0.025 I				4,400		0.085	5	20500	25800	X	300	
FLUOMETURON	2164-17-2	0.013 I				68		97.5	2,5,6,8					
FLUORANTHENE	206-44-0	0.04 I		0.04 Ir		49000		0.26	1,5,6				375	0.29
FLUORENE	86-73-7	0.04 I		0.04 Ir		7900		1.9	1				298	2.11
FLUOROTRICHLOROMETHANE (FREON 11)	75-69-4	0.3 I		0.2 H		130	X	1090	1,4,5,6	13100	15000	X	24	0.35
FONOFOS	944-22-9	0.002 I		0.002 Ir		1100	X	13	5,6,8	13400	15500	X	130	
FORMALDEHYDE	50-00-0	0.2 I	0.0455 Ir	0.0011 D	0.0455 I	3.6	X	55000	1	13100	15100	X	-21	18.07
FORMIC ACID	64-18-6	2 H		2 Hr		0.54	X	1000000	2	13000	14900	X	101	18.07
FOSETYL-AL	39148-24-8	3 I				310		120000	2					
FURAN	110-00-9	0.001 I				130	X	10000	1	13100	15000	X	31.36	2.25
FURFURAL	98-01-1	0.003 I		0.0143 H		6.3	X	91000	1,2,3	13000	14900	X	162	
GLYPHOSATE	1071-83-6	0.1 I		0.1 Ir		3500		12000	1,5,6				186	
HEPTACHLOR	76-44-8	0.0005 I	4.5 I	0.0005 Ir	4.55 I	6800		0.18	4,6,7				310	46.84
HEPTACHLOR EPOXIDE	1024-57-3	0.000013 I	9.1 I	0.000013 Ir	9.1 I	21000		0.311	4,6,7,9				200	0.23
HEXACHLOROAZOBENZENE	118-74-1	0.0008 I	1.6 I	0.0008 Ir	1.61 I	3800		0.006	1,4,5				319	0.06
HEXACHLOROBUTADIENE	87-68-3	0.0002 H	0.078 I	0.0002 Hr	0.077 I	4700		2.89	4,5,6,7			X	215	0.69
HEXACHLOROCYCLOPENTADIENE	77-47-4	0.006 I		0.00006 H		7200		1.8	5,6,7			X	239	4.50
HEXACHLOROETHANE	67-72-1	0.001 I	0.014 I	0.001 Ir	0.014 I	2200		50	1				187	0.69
HEXANE	110-54-3	0.06 H		0.0571 I		3600	X	9.5	1,5,6	13100	15000	X	69	
HEXYTHIAZOX (SAVEY)	78587-05-0	0.025 I				6,500		0.5	2					
HYDRAZINE/HYDRAZINE SULFATE	302-01-2		3 I		17 I	0.0053	X	1000000	2	13000	15000	X	113.5	18.07
HYDROQUINONE	123-31-9	0.04 H		0.04 Hr		10		70000	2,3,5				285	18.07
INDENO[1,2,3-CD]PYRENE	193-39-5		0.73 N		0.31 T	31000000		0.062	5				536	0.17
IPRODIONE	36734-19-7	0.04 I				1,100		13	2					
ISOBUTYL ALCOHOL	78-83-1	0.3 I		0.3 Ir		60	X	81000	1,2,3,4,5	13000	14900	X	108	17.57
ISOPHORONE	78-59-1	0.2 I	0.00095 I	0.2 Ir	0.00095 Ir	31		12000	2,4,5			X	215	4.50
KEPONE	143-50-0	0.0005 D	16 C		16.1 C	55000		7.6	4				350	0.17
MALATHION	121-75-5	0.02 I		0.02 Ir		1300	X	143	4	14000	16300	X	157	2.46
MALEIC HYDRAZIDE	123-33-1	0.5 I		0.5 Ir		2.8		6000	4				260	

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Appendix A
Table 5 - Physical and Toxicological Properties
A. Organic Regulated Substances

Regulated Substance	CAS	RfDo (mg/kg-d)	CSFo (mg/kg-d)-1	RfDi (mg/kg-d)	CSFi (mg/kg-d)-1	Koc	VOC?	Aqueous Sol (mg/L)	Aqueous Sol Reference ¹	TF Vol from Surface Soil	TF Vol from SubSurface Soil	Organic Liquid	Boiling Point (degrees C)	Degradation Coefficient (K/yr ¹)
MANEB	12427-38-2	0.005 I				1		23	9.13					
MERPHOS OXIDE	78-48-8	0.00003 I				53,000	X	2.3	8.10,12	13100	15100	X	150	
METHACRYLONITRILE	126-98-7	0.0001 I		0.0002 H		21	X	25700	1	13100	15100	X	90	
METHAMIDOPHOS	10265-92-6	0.00005 I				5		2000000	5					
METHANOL	67-56-1	0.5 I		0.5 Ir		2.8	X	1000000	2	13100	15100	X	65	36.14
METHOMYL	16752-77-5	0.025 I		0.025 Ir		20		58000	2				144	
METHOXYCHLOR	72-43-5	0.005 I		0.005 Ir		63000		0.045	4.5,6				346	0.69
METHOXYETHANOL, 2-	109-86-4	0.001 H		0.00571 I			X	1000000	2	13100	15000	X	124.3	4.50
METHYL ACETATE	79-20-9	1 H				30	X	243500	4.5,6	13100	15100	X	56.9	
METHYL ACRYLATE	96-33-3	0.03 H				55	X	52000	1.2,5	13100	15100	X	70	18.07
METHYL CHLORIDE	74-87-3	0.004 M	0.013 H	0.029 D	0.0063 H	6	X	6180	1.2,3,4	13200	15000	X	-24	4.50
METHYL ETHYL KETONE	78-93-3	0.6 I		0.286 I		32	X	275000	1.2,3,4,5	13100	15100	X	80	2.57
METHYL ISOBUTYL KETONE	108-10-1	0.08 H		0.023 H		17	X	19550	1.2,4,5	13100	15100	X	117	18.07
METHYL METHACRYLATE	80-62-6	1.4 I		0.2 I		10	X	15600	1	13100	15100	X	100	4.5045
METHYL METHANESULFONATE	66-27-3		0.099 C		0.098 C	5.2		200000	2				203	
METHYL PARATHION	298-00-0	0.00025 I		0.00025 Ir		790	X	25	4.5,6	13500	15600	X	133	3.61
METHYL STYRENE (MIXED ISOMERS)	25013-15-4	0.006 H		0.011 H		2,200		89	9					
METHYL TERT-BUTYL ETHER (MTBE)	1634-04-4	0.857 Ir	0.0018 C	0.857 I	0.0018 C	12	X	45000	1.2,4,6	13100	15100	X	55	0.693
METHYLENE BIS(2-CHLOROANILINE), 4,4'-	101-14-4	0.0007 H	0.13 H	0.0007 Hr	0.13 H	3,000		13.9	10					
METHYLNAPHTHALENE, 2-	91-57-6	0.02 S		0.00086 S		16000		25	1			X	241	
METHYLSTYRENE, ALPHA	98-83-9	0.07 H				660	X	560	9			X	165.4	
NAPHTHALENE	91-20-3	0.02 I		0.00086 I		950		30	3				218	0.98
NAPHTHYLAMINE, 1-	134-32-7		1.8 S		1.8 S	3200		1690	2				301	0.69
NAPHTHYLAMINE, 2-	91-59-8		1.8 C		1.8 C	87		6.4	6				306	0.69
NAPROPAMIDE	15299-99-7	0.1 I				880		70	2					
NITROANILINE, M-	99-09-2	0.0000571 S		0.0000571 S		18		100	3				306	
NITROANILINE, O-	88-74-4	0.0000571 Hr		0.0000571 H		27		1200	6				284	
NITROANILINE, P-	100-01-6	0.0000571 S		0.0000571 S		15		800	2				332	
NITROBENZENE	98-95-3	0.0005 I		0.0006 H		130		2000	2			X	211	0.64
NITROPHENOL, 2-	88-75-5	0.008 S		0.008 S		37		2100	1.2,3,4,5,6				215	9.01
NITROPHENOL, 4-	100-02-7	0.008 N		0.008 Nr		230		16000	2				279	25.81
NITROPROPANE, 2-	79-46-9	0.00571 Ir	9.4 Hr	0.00571 I	9.4 H	20	X	16700	1.3,4,5	13000	14900	X	120	0.69
NITROSODIETHYLAMINE, N-	55-18-5		150 I		151 I	26	X	93000	10	13000	14900	X	176	0.69
NITROSODIMETHYLAMINE, N-	62-75-9		51 I		49 I	8.5	X	1000000	2	13000	14900	X	154	0.69
NITROSO-DI-N-BUTYLAMINE, N-	924-16-3		5.4 I		5.6 I	450		1200	0.13			X	235	0.69
NITROSODI-N-PROPYLAMINE, N-	621-64-7	0.095 D	7 I	0.095 Dr	7 C	11		9900	6			X	206	0.69
NITROSODIPHENYLAMINE, N-	86-30-6		0.0049 I		0.0091 C	580		35	1				269	3.72
NITROSO-N-ETHYLUREA, N-	759-73-9		140 H		27 C	2		13000	9				125	1734.48
OCTYL PHTHALATE, DI-N-	117-84-0	0.02 H		0.02 Hr		980000000		3	5			X	234	0.69
OXAMYL (VYDATE)	23135-22-0	0.025 I		0.025 Ir		7.1		280000	2				101	
PARATHION	56-38-2	0.006 H		0.006 Hr		2300		20	2,4,5,6,7			X	375	
PCB-1016 (AROCLOR)	12674-11-2	0.00007 I	0.09 N	0.00007 Ir	0.09 Nr	110000		0.25	5			X	340	
PCB-1221 (AROCLOR)	11104-28-2		0.5 S		0.5 S	1900		0.59	5			X	340	
PCB-1232 (AROCLOR)	11141-16-5		0.5 S		0.5 S	1500		1.45	7			X	340	
PCB-1242 (AROCLOR)	53469-21-9		0.5 N		0.5 Nr	48000		0.1	5			X	340	
PCB-1248 (AROCLOR)	12672-29-6		1.8 S		1.8 S	190000		0.054	7.9,11			X	340	
PCB-1254 (AROCLOR)	11097-69-1	0.00002 I	1.8 N	0.00002 Ir	1.8 Nr	810000		0.057	5			X	340	
PCB-1260 (AROCLOR)	11096-82-5		0.6 N		0.6 Nr	1800000		0.08	5				385	
PEBULATE	1114-71-2	0.05 H				630	X	92	5	13000	14900	X	142	
PENTACHLOROBENZENE	608-93-5	0.0008 I		0.0008 Ir		32000		0.74	1.5,6,7				277	0.37
PENTACHLORONITROBENZENE	82-68-8	0.003 I	0.26 H	0.003 Ir	0.26 Hr	7900		0.44	4.6,8				328	0.36
PENTACHLOROPHENOL	87-86-5	0.03 I	0.12 I	0.03 Ir	0.12 Ir	20000		14	1.2,4,5				310	0.17
PHENACETIN	62-44-2		0.0022 C		0.0022 C	110		763	2.3,9				200	4.50
PHENANTHRENE	85-01-8	0.3 S		0.3 Sr		38000		1.1	1.4,5				341	0.63
PHENOL	108-95-2	0.6 I		0.6 Ir		22	X	84300	1.2,3,4			X	182	36.14
PHENYLENEDIAMINE, M-	108-45-2	0.006 I		0.006 Ir		12		351000	3				286	4.50
PHENYLPHENOL, 2-	90-43-7		0.00194 H			5,700		700	5				280	18.07
PHORATE	298-02-2	0.0002 H		0.0002 Hr		810	X	50	2	13100	15100	X	118	
PHTHALIC ANHYDRIDE	85-44-9	2 I		0.0343 H		79		6170	2				285	13490.40
PICLORAM	1918-02-1	0.07 I				15		430	2					
POLYCHLORINATED BIPHENYLS (AROCLORS) (PCBS)	1336-36-3		2 I		2 I			0.0505	10,13					
PRONAMIDE	23950-58-5	0.075 I		0.075 Ir		200		15	2				321	
PROPANIL	709-98-8	0.005 I				160		225	2					
PROPHAM	122-42-9	0.02 I				51		250	5					
PROPYLBENZENE, N-	103-65-1	0.04 N				720	X	52	6	13100	15100	X	159.2	
PROPYLENE OXIDE	75-56-9	0.00857 Ir	0.24 I	0.00857 I	0.013 I	25	X	405000	1	13100	15000	X	34	
PYRENE	129-00-0	0.03 I		0.03 Ir		68000		0.132	1				393	0.07
PYRIDINE	110-86-1	0.001 I		0.001 Ir		0.0066	X	1000000	2	13100	15000	X	115	18.07

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QUINOLINE	91-22-5		12 H			1,300		60000	1,3,5		14900	X	237.7	12.65
QUIZALOFOP (ASSURE)	76578-14-8	0.009 I				580		0.3	2				220	
RONNEL	299-84-3	0.05 H				580		40	2				151	
SIMAZINE	122-34-9	0.005 I	0.12 H	0.005 Ir	0.12 Hr	110		5	5				225	
STRYCHNINE	57-24-9	0.0003 I		0.0003 Ir		280		143	5				270	4.50
STYRENE	100-42-5	0.2 I		0.286 I		910	X	300	5	13100	15100	X	145	1.20
TEBUTHIURON	34014-18-1	0.07 I				620		2500	2					
TERBACIL	5902-51-2	0.013 I				53		710	2					
TERBUFOS	13071-79-9	0.00025 H		0.000025 Hr		510	X	5	6	13000	15000	X	69	
TETRACHLORO BENZENE, 1,2,4,5-	95-94-3	0.0003 I		0.0003 Ir		1,800		0.583	1,5,6,7				245	0.69
TETRACHLORODIBENZO-P-DIOXIN, 2,3,7,8- (TCDD)	1746-01-6	0.000000001 D	150000 H		150000 H	4300000		0.0000193	6				412	0.21
TETRACHLOROETHANE, 1,1,1,2-	630-20-6	0.03 I	0.026 I	0.03 Ir	0.0259 I	980	X	1100	1			X	130.5	3.79
TETRACHLOROETHANE, 1,1,2,2-	79-34-5	0.06 N	0.2 I	0.06 Nr	0.203 I	79	X	2860	2	13100	15100	X	147	0.56
TETRACHLOROETHYLENE (PCE)	127-18-4	0.01 I	0.052 N	0.14 N	0.00203 N	300	X	182	1,2,3,4,5	13100	15000	X	121	0.03
TETRACHLOROPHENOL, 2,3,4,6-	58-90-2	0.03 I		0.03 Ir		6200		183	6				150	0.69
TETRAETHYL LEAD	78-00-2	0.0000001 I		0.0000001 Ir		4900		0.8	5			X	200	4.50
TETRAETHYLDITHIOPYROPHOSPHATE	3689-24-5	0.0005 I		0.0005 Ir		550	X	25	2	13000	14900	X	136	
THIOFANOX	39196-18-4	0.0003 H				0.022		5200	9					
THIRAM	137-26-8	0.005 I		0.005 Ir		1000		30	4				200	
TOLUENE	108-88-3	0.2 I		0.114 I		130	X	532.4	1,2,3,4	13100	15000	X	111	9.01
TOLUIDINE, M-	108-44-1		0.24 S		0.24 Sr	140		15030	6			X	203	
TOLUIDINE, O-	95-53-4		0.24 H		0.24 Hr	410		15000	1,3,5			X	200	18.07
TOLUIDINE, P-	106-49-0		0.19 H		0.19 Hr	320		7410	1,2,3				200	
TOXAPHENE	8001-35-2	0.001 D	1.1 I	0.001 Dr	1.12 I	1500		3	2,4,5				432	
TRIALATE	2303-17-5	0.013 I				2,000		4	5				117	
TRIBROMOMETHANE (BROMOFORM)	75-25-2	0.02 I	0.0079 I	0.02 Ir	0.00385 I	130	X	3050	1,2,3,4	13100	15100	X	149	0.69
TRICHLORO-1,2,2-TRIFLUOROETHANE, 1,1,2-	76-13-1	30 I		8.57 H		1,200	X	170	1			X	47.7	0.35
TRICHLORO BENZENE, 1,2,4-	120-82-1	0.01 I	0.0036 C	0.0571 H		1500		44.4	1,4,6,7			X	213	0.69
TRICHLORO BENZENE, 1,3,5-	108-70-3	0.006 M		0.0571 S		3100		5.8	5				208	
TRICHLOROETHANE, 1,1,1-	71-55-6	0.28 N		0.63 N		100	X	1495	1,4,5,6	13100	15000	X	74	0.05
TRICHLOROETHANE, 1,1,2-	79-00-5	0.004 I	0.057 I	0.004 Ir	0.056 I	76	X	4420	1	13100	15100	X	114	0.03
TRICHLOROETHYLENE (TCE)	79-01-6	0.006 N	0.011 N	0.143 D	0.00595 N	93	X	1100	1	13100	15000	X	87	0.02
TRICHLOROPHENOL, 2,4,5-	95-95-4	0.1 I		0.1 Ir		2400		1000	1,2,4				246	0.14
TRICHLOROPHENOL, 2,4,6-	88-06-2	0.0003 I	0.011 I	0.0003 I	0.01085 I	1100		850	1,2,4,5				246	0.14
TRICHLOROPHENOXYACETIC ACID, 2,4,5- (2,4,5-T)	93-76-5	0.01 I		0.01 Ir		43		278	2,4,5				279	1.39
TRICHLOROPHENOXYPROPIONIC ACID, 2,4,5- (2,4,5-TP)(SILVEX)	93-72-1	0.008 I		0.008 Ir		1700		140	2				200	
TRICHLOROPROPANE, 1,1,2-	598-77-6	0.005 I				24	X	2700	14	13100	15000	X	117	
TRICHLOROPROPANE, 1,2,3-	96-18-4	0.006 I	7 H	0.0014 N	7 Hr	280	X	1896	1,4,6	13100	15100	X	157	0.35
TRICHLOROPROPENE, 1,2,3-	96-19-5	0.005 H				190	X	2700	14	13100	15000	X	142	
TRIFLURALIN	1582-09-8	0.0075 I	0.0077 I	0.0075 Ir	0.0077 Ir	720		4	2,5,6,7				139	
TRIMETHYLBENZENE, 1,3,4- (TRIMETHYLBENZENE, 1,2,4-)	95-63-6	0.05 N		0.0017 N		2,200	X	56	1	13100	15000	X	169	4.50
TRIMETHYLBENZENE, 1,3,5-	108-67-8	0.05 N		0.0017 N		660	X	48.9	1	13100	15100	X	164.7	
TRINITROTOLUENE, 2,4,6-	118-96-7	0.0005 I	0.03 I			1		100	2				240	
VINYL ACETATE	108-05-4	1 I		0.0571 I		2.8	X	20000	1	13200	15000	X	73	
VINYL BROMIDE (BROMOETHENE)	593-60-2	0.000857 Ir	0.11 Hr	0.000857 I	0.11 H	150		4180	12				15.8	0.09
VINYL CHLORIDE	75-01-4	0.003 I	1.5 I	0.029 I	0.03 I	10	X	2700	1	13200	15000	X	-13	0.09
WARFARIN	81-81-2	0.0003 I		0.0003 Ir		910		17	4				356	4.50
XYLENES (TOTAL)	1330-20-7	2 I		0.12 D		350	X	175	13	13100	15000	X	140	0.69
ZINEB	12122-67-7	0.05 I				19		10	4					

Toxicity Value Sources:

C = California EPA Cancer Potency Factor

D = ATSDR Minimal Risk Level

H = Health Effects Assessment Summary Table (HEAST)

I = Integrated Risk information System (IRIS)

M = EPA Drinking Water Regulations and Health Advisories

N = EPA NCEA Provisional Values

r = route-to-route extrapolation

¹ Aqueous solubility references are keyed to the numbered list found at 250.304(f). Where there are multiple sources cited, the table value is the median of the values in the individual references.

APENDIX A
Table 5 - Physical and Toxicological Properties
B. Inorganic Regulated Substances

Regulated Substance	CAS	RfDo (mg/kg-d)	CSFo (mg/kg-d)-1	RfDi (mg/kg-d)	CSFi (mg/kg-d)-1	Kd
ALUMINUM	7429-90-5	1 N		0.001 N		
ANTIMONY	7440-36-0	0.0004 I		0.0004 lr		45
ARSENIC	7440-38-2	0.0003 I	1.5 I	0.0003 lr	15 I	29
BARIUM AND COMPOUNDS	7440-39-3	0.07 I		0.0001 H		41
BERYLLIUM	7440-41-7				8.4 I	790
BORON AND COMPOUNDS	7440-42-8	0.09 I		0.0057 H		
CADMIUM	7440-43-9	0.0005 I	0.38 C	0.0005 lr	6.3 I	75
CHROMIUM III	16065-83-1	1.5 I				1800000
CHROMIUM VI	18540-29-9	0.003 I	0.19 C	0.00003 I	42 I	19
COBALT	7440-48-4	0.02 N		0.000005 D		
COPPER	7440-50-8	0.0371 H				360
CYANIDE, TOTAL	57-12-5	0.02 I		0.02 lr		9.9
IRON	7439-89-6	0.3 N		0.3 Nr		
LEAD	7439-92-1		0.0085 C		0.042 C	890
MANGANESE	7439-96-5	0.14 I		0.0000143 I		
MERCURY	7439-97-6	0.0003 M		0.000086 I		52
NICKEL	7440-02-0	0.02 I		0.0000571 D	0.84 Is	65
SELENIUM	7782-49-2	0.005 I		0.005 lr		5
SILVER	7440-22-4	0.005 I		0.005 lr		8.3
THALLIUM	7440-28-0	0.00007 I		0.00007 lr		71
TIN	7440-31-5	0.6 H		0.6 Hr		
VANADIUM	7440-62-2	0.007 H		0.000057 D		1000
ZINC	7440-66-6	0.3 I		0.3 lr		62

Toxicity Value Sources:

C = California EPA Cancer Potency Factor

D = ATSDR Minimal Risk Level

H = Health Effects Assessment Summary Table (HEAST)

I = Integrated Risk information System (IRIS)

M = EPA Drinking Water Regulations and Health Advisories

N = EPA NCEA Provisional Values

r = route-to-route extrapolation

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Parameters for Assessing Transport
of Environmentally Released
Radionuclides through Agriculture**

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R. D. Sharp
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R. W. Shor

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Health and Safety Research Division

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Date Published: September 1984

Research sponsored by the Office of Radiation Programs, U. S. Environmental Protection Agency under Interagency Agreement AD-89-F-2-A106 (formerly EPA-78-D-X0394).

Prepared by the
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
operated by
Martin Marietta Energy Systems, Inc.
for the
U. S. DEPARTMENT OF ENERGY
under contract No. DE-AC05-84OR21400

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MASTER

I A II A		III B IV B V B VI B VII B VIII I B II B										III A IV A V A VI A VII A						
II	Li 300	Be 650											B 3.0	M 0.50		F 150		
III	Na 100	Mg 4.5											Al 1500	S 7.5	Cl 0.25			
IV	K 5.5	Ca 4.0	Sc 1000	Ti 1000	V 1000	Cr 850	Mn 65	Fe 25	Co 45	Ni 150	Cu 35	Zn 40	Ga 1500	Ge 25	As 200	Se 300	Br 7.5	
V	Rb 60	Sr 35	Y 500	Zr 3000	Nb 350	Mo 20	Tc 1.5	Ru 350	Rh 60	Pd 60	Ag 45	Cd 6.5	In 1500	Sn 250	Sb 45	Te 300	I 60	
VI	Cs 1000	Ba 60		Hf 1500	Ta 650	W 150	Re 7.5	Os 450	Ir 150	Pt 90	Au 25	Hg 10	Tl 1500	Pb 900	Bi 200	Po 500	At 10	
VII	Fr 250	Ra 450																
Lanthanides			La 650	Ce 850	Pr 650	Nd 650	Pm 650	Sm 650	Eu 650	Gd 650	Tb 650	Dy 650	Ho 650	Er 650	Tm 650	Yb 650	Lu 650	
Actinides			Ac 1500	Th 1.5x10 ⁵	Pa 2500	U 450	Np 30	Pu 4500	Am 700	Cm 2000								
Key:			LI	Symbol														
			300	Transfer Coefficient, K _d														

Figure 2.31. Values of the soil-water distribution coefficient K_d adopted as default estimates in the computer code TERRA.

HANDBOOK OF

PHYSICAL
PROPERTIES
OF
ORGANIC
CHEMICALS

Edited by

Philip H. Howard and William M. Meylan

*Environmental Sciences Center
Syracuse Research Corporation*

Associate Editors

Julie Funk, Michelle Pepling, Gloria W. Sage,
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LEWIS PUBLISHERS

Boca Raton New York London Tokyo

Acquiring Editor: Joel Stein
Marketing Manager: Greg Daurelle
Direct Marketing Manager: Arline Massey
Cover design: Jonathan Pennell
Manufacturing: Sheri Schwartz

Library of Congress Cataloging-in-Publication Data

Catalog record is available from the Library of Congress

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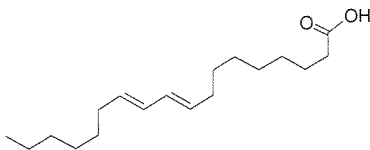
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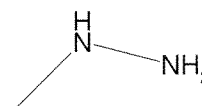
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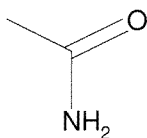
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Formula: $C_{18}H_{32}O_2$			
Mol Weight: 280.45			
MP (deg C): -12		FP (deg C):	
BP (deg C): 230			
BP pressure (mm Hg): 1.60E+001			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	25	EST MEYLAN,WM ET AL. (1996)
logP			EXP SANGSTER,J (1993)
VP	mm Hg	25	EXP DAUBERT,TE & DANNER,RP (1989)
DC	pKa	25	EXP SERJEANT,EP & DEMPSEY,B (1979)
HL	atm m ³ /mol	25	EST MEYLAN,WM & HOWARD,PH (1991)
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)



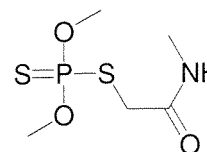
CAS #:		METHYL HYDRAZINE	
Formula: CH_6N_2			
Mol Weight: 46.07			
MP (deg C): -52.4		FP (deg C):	
BP (deg C): 87.5			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L		EXP MERCK INDEX (1983)
logP			EXP HANSCH,C ET AL. (1995)
VP	mm Hg	25	EXP BOUBLIK,T ET AL. (1984)
DC	pKa	30	EXP PERRIN,DD (1965)
HL	atm m ³ /mol	25	EST VP/WSOL
OH	cm ³ /molc sec	25	EXP ATKINSON,R (1989)



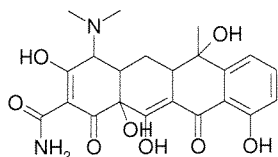
CAS #:		ACETAMIDE	
Formula: C_2H_5NO			
Mol Weight: 59.07			
MP (deg C): 69.5		FP (deg C):	
BP (deg C): 221.15			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	25	EXP YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP			EXP HANSCH,C & LEO,AJ (1985)
VP	mm Hg	25	EST NEELY,WB & BLAU,GE (1985)
DC	pKa		EXP WEAST,RC (1972)
HL	atm m ³ /mol	25	EST MEYLAN,WM & HOWARD,PH (1991)
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)



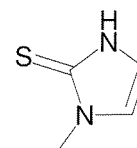
CAS #:		DIMETHOATE	
Formula: $C_5H_{12}NO_3PS_2$			
Mol Weight: 229.26			
MP (deg C): 52-52.5		FP (deg C):	
BP (deg C): 107			
BP pressure (mm Hg): 5.00E-002			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	20	EXP TOMLIN,C (1994)
logP			EXP HANSCH,C ET AL. (1995)
VP	mm Hg	25	EXP TOMLIN,C (1994)
DC	pKa		
HL	atm m ³ /mol	25	EST VP/WSOL
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)



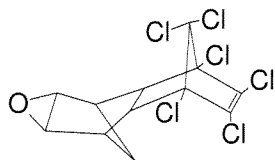
CAS #:		TETRACYCLINE	
Formula: $C_{22}H_{24}N_2O_8$			
Mol Weight: 444.45			
MP (deg C): 170-175 de		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	25	EXP YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP			EXP HANSCH,C & LEO,AJ (1985)
VP	mm Hg	25	EST NEELY,WB & BLAU,GE (1985)
DC	pKa	25	EXP KORTUM,G ET AL (1961)
HL	atm m ³ /mol	25	EST MEYLAN,WM & HOWARD,PH (1991)
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)



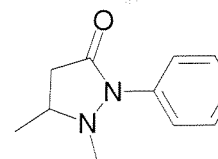
CAS #:		METHIMAZOLE	
Formula: $C_4H_6N_2S$			
Mol Weight: 114.17			
MP (deg C): 146-148		FP (deg C):	
BP (deg C): 280			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	25	EST MEYLAN,WM ET AL. (1996)
logP			EXP HANSCH,C ET AL. (1995)
VP	mm Hg	25	EST NEELY,WB & BLAU,GE (1985)
DC	pKa		
HL	atm m ³ /mol	25	EST MEYLAN,WM & HOWARD,PH (1991)
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)

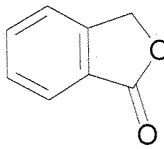


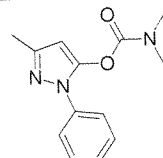
CAS #:		DIELDRIN	
Formula: $C_{12}H_8Cl_6O$			
Mol Weight: 380.91			
MP (deg C): 175-176		FP (deg C):	
BP (deg C): 330			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	25	EXP BIGGAR,JW & RIGGS,RI (1974)
logP			EXP DEBRUIJN,J ET AL. (1989)
VP	mm Hg	25	EXP GRAYSON,BT & FOSBRAEY,LA (1982)
DC	pKa		
HL	atm m ³ /mol	25	EXP WARNER,HP ET AL. (1987)
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)

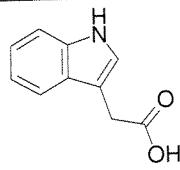


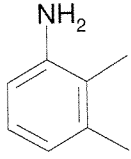
CAS #:		ANTIPYRINE	
Formula: $C_{11}H_{14}N_2O$			
Mol Weight: 190.25			
MP (deg C): 111-113		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type Reference
WS	mg/L	25	EXP YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP			EXP HANSCH,C & LEO,AJ (1985)
VP	mm Hg	25	EST NEELY,WB & BLAU,GE (1985)
DC	pKa		
HL	atm m ³ /mol	25	EST MEYLAN,WM & HOWARD,PH (1991)
OH	cm ³ /molc sec	25	EST MEYLAN,WM & HOWARD,PH (1993)

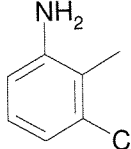


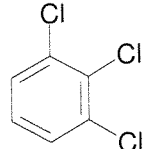
CAS #		000087-41-2		PHTHALIDE		
Formula:		$C_8H_6O_2$				
Mol Weight:		134.14				
MP (deg C):	75	FP (deg C):				
BP (deg C):		290				
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	1.84E+004	mg/L	25	EST	MEYLAN,WM ET AL. (1996)	
logP	0.80			EXP	HANSCH,C & LEO,AJ (1985)	
VP	7.07E-003	mm Hg	25	EXT	PERRY,RH & GREEN,D (1984)	
DC		pKa				
HL	1.27E-005	atm m3/mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)	
OH	2.76E-012	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

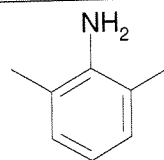
CAS #		000087-47-8		PYROLAN		
Formula:		$C_{13}H_{15}N_3O_2$				
Mol Weight:		245.28				
MP (deg C):	50	FP (deg C):				
BP (deg C):		160-162				
BP pressure (mm Hg):		2.00E-001				
Property/Value	Units	Temp	Data Type	Reference		
WS	2.00E+003	mg/L		EXP	YALKOWSKY,SH & DANNENFELSER,RM (1992)	
logP	1.96			EST	MEYLAN,WM & HOWARD,PH (1995)	
VP	7.77E-006	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)	
DC		pKa				
HL	1.94E-013	atm m3/mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)	
OH	1.17E-010	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

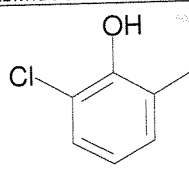
CAS #		000087-51-4		INDOLE-3-ACETIC ACID		
Formula:		$C_{10}H_9NO_2$				
Mol Weight:		175.19				
MP (deg C):	168-170	FP (deg C):				
BP (deg C):						
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	1.50E+003	mg/L	25	EXP	SHIU,WY ET AL. (1990)	
logP	1.41			EXP	HANSCH,C & LEO,AJ (1985)	
VP	5.26E-006	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)	
DC		pKa				
HL	7.27E-012	atm m3/mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)	
OH	1.84E-010	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

CAS #		000087-59-2		2,3-DIMETHYLANILINE		
Formula:		$C_8H_{11}N$				
Mol Weight:		121.18				
MP (deg C):	2.5	FP (deg C):				
BP (deg C):		221.5				
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	1.39E+003	mg/L	25	EST	MEYLAN,WM ET AL. (1996)	
logP	2.17			EST	MEYLAN,WM & HOWARD,PH (1995)	
VP	7.50E-002	mm Hg	25	EXP	WEBER,RC ET AL. (1981)	
DC	4.70	pKa	25	EXP	PERRIN,DD (1965)	
HL	2.32E-006	atm m3/mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)	
OH	2.00E-010	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

CAS #		000087-60-5		2-METHYL-3-CHLOROANILINE		
Formula:		C_7H_8ClN				
Mol Weight:		141.60				
MP (deg C):	1	FP (deg C):				
BP (deg C):		245				
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	9.54E+002	mg/L	25	EST	MEYLAN,WM ET AL. (1996)	
logP	2.27			EST	MEYLAN,WM & HOWARD,PH (1995)	
VP	4.08E-002	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)	
DC		pKa				
HL	1.56E-006	atm m3/mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)	
OH	1.20E-010	cm3/mol sec	25	EST	ATKINSON,R (1987)	

CAS #		000087-61-6		1,2,3-TRICHLOROBENZENE		
Formula:		$C_6H_3Cl_3$				
Mol Weight:		181.45				
MP (deg C):	52.6	FP (deg C):				
BP (deg C):		221				
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	1.80E+001	mg/L	25	EXP	CHIOU,CT ET AL. (1986)	
logP	4.05			EXP	SANGSTER,J (1994)	
VP	2.10E-001	mm Hg	25	EXP	MACKAY,D ET AL. (1982)	
DC		pKa				
HL	1.25E-003	atm m3/mol	25	EXP	MACKAY,D ET AL. (1982A)	
OH	2.91E-013	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

CAS #		000087-62-7		2,6-DIMETHYLANILINE		
Formula:		$C_8H_{11}N$				
Mol Weight:		121.18				
MP (deg C):	11.2	FP (deg C):				
BP (deg C):		215				
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	8.24E+003	mg/L	25	EXP	HUYSKENS,P ET AL. (1975)	
logP	2.17			EST	MEYLAN,WM & HOWARD,PH (1995)	
VP	1.30E-001	mm Hg	25	EXP	CHAO,J ET AL. (1983)	
DC	3.95	pKa	25	EXP	HUYSKENS,P ET AL. (1975)	
HL	2.52E-006	atm m3/mol	25	EST	VP/WSOL	
OH	1.95E-010	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

CAS #		000087-64-9		2-METHYL-6-CHLOROPHENOL		
Formula:		C_7H_7ClO				
Mol Weight:		142.59				
MP (deg C):		FP (deg C):				
BP (deg C):		189				
BP pressure (mm Hg):						
Property/Value	Units	Temp	Data Type	Reference		
WS	1.26E+003	mg/L	25	EST	MEYLAN,WM ET AL. (1996)	
logP	2.80			EXP	SOTOMATSU,T ET AL. (1993)	
VP	4.05E-002	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)	
DC	8.69	pKa	20	EXP	SERJEANT,EP & DEMPSEY,B (1979)	
HL	4.58E-007	atm m3/mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)	
OH	1.22E-011	cm3/mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)	

CAS #		IODOBENZENE	
Formula:		<chem>C6H5I</chem>	
Mol Weight:		204.01	
MP (deg C):	-30	FP (deg C):	
BP (deg C):	188-189		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	3.40E+002	mg/L	30 EXP
logP	3.25		EXP
VP	1.06E+000	mm Hg	25 EXP
DC		pKa	
HL	8.37E-004	atm m ³ /mol	25 EST
OH	1.10E-012	cm ³ /mol·sec	25 EXP

CAS #		4-PYRIDINAMINE	
Formula:		<chem>C4H5N3</chem>	
Mol Weight:		95.10	
MP (deg C):	154-156	FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.97E+005	mg/L	25 EST
logP	-0.25		EXP
VP	2.46E-001	mm Hg	25 EST
DC	5.69	pKa	20 EXP
HL	1.03E-009	atm m ³ /mol	25 EST
OH	1.27E-011	cm ³ /mol·sec	25 EST

CAS #		2-METHYLHEXANE	
Formula:		<chem>C7H16</chem>	
Mol Weight:		100.21	
MP (deg C):	-118.2	FP (deg C):	
BP (deg C):	90		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	2.54E+000	mg/L	25 EXP
logP	3.71		EST
VP	6.60E+001	mm Hg	25 EXP
DC		pKa	
HL	3.43E+000	atm m ³ /mol	25 EST
OH	6.86E-012	cm ³ /mol·sec	25 EST

CAS #		2-HEXANONE	
Formula:		<chem>C6H12O</chem>	
Mol Weight:		100.16	
MP (deg C):	-55.5	FP (deg C):	
BP (deg C):	127.6		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.75E+004	mg/L	20 EXP
logP	1.38		EXP
VP	1.16E-001	mm Hg	25 EXP
DC		pKa	
HL	8.74E-007	atm m ³ /mol	25 EST
OH	9.10E-012	cm ³ /mol·sec	25 EXP

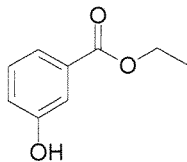
CAS #		PROPANE, 1-ISOTHIOCYANATO-2-METHYL-	
Formula:		<chem>C5H9NS</chem>	
Mol Weight:		115.20	
MP (deg C):		FP (deg C):	
BP (deg C):	160		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	4.08E+002	mg/L	25 EST
logP	2.82		EXP
VP	4.73E+000	mm Hg	25 EST
DC		pKa	
HL	7.27E-003	atm m ³ /mol	25 EST
OH	3.87E-012	cm ³ /mol·sec	25 EST

CAS #		ALLYL ACETATE	
Formula:		<chem>C5H8O2</chem>	
Mol Weight:		100.12	
MP (deg C):		FP (deg C):	
BP (deg C):	103.5		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.74E+004	mg/L	25 EST
logP	0.97		EXP
VP	3.52E+001	mm Hg	25 EXP
DC		pKa	
HL	2.30E-004	atm m ³ /mol	25 EST
OH	2.79E-011	cm ³ /mol·sec	25 EST

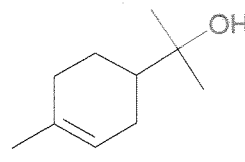
CAS #		1,4-PENTADIENE	
Formula:		<chem>C5H8</chem>	
Mol Weight:		68.12	
MP (deg C):	-148.8	FP (deg C):	
BP (deg C):	26		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	5.58E+002	mg/L	25 EXP
logP	2.48		EXP
VP	7.48E+002	mm Hg	25 EXP
DC		pKa	
HL	1.20E-001	atm m ³ /mol	25 EST
OH	5.33E-011	cm ³ /mol·sec	25 EXP

CAS #		1,2-PENTADIENE	
Formula:		<chem>C5H8</chem>	
Mol Weight:		68.12	
MP (deg C):	-137.3	FP (deg C):	
BP (deg C):	44.9		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	2.61E+002	mg/L	25 EST
logP	2.55		EST
VP	3.68E+002	mm Hg	25 EXP
DC		pKa	
HL	1.28E-001	atm m ³ /mol	25 EST
OH	3.55E-011	cm ³ /mol·sec	25 EXP

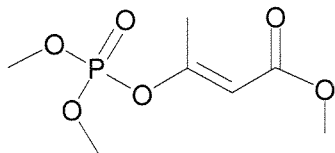
CAS #:		ETHYL-3-HYDROXYBENZOATE	
Formula:		$C_9H_{10}O_3$	
Mol Weight:		166.18	
MP (deg C):	74	FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.89E+003	mg/L	25 EST
logP	2.47		EXP SANGSTER,J (1993)
VP	1.73E-003	mm Hg	25 EST
DC		pKa	NEELY,WB & BLAU,GE (1985)
HL	4.79E-009	atm m ³ /mol	25 EST
OH	9.33E-012	cm ³ /mol sec	25 EST



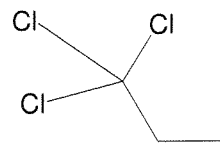
CAS #:		D-ALPHA-TERPINEOL	
Formula:		$C_{10}H_{18}O$	
Mol Weight:		154.25	
MP (deg C):		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	6.70E+002	mg/L	25 EST
logP	3.33		EST MEYLAN,WM & HOWARD,PH (1995)
VP	3.07E-002	mm Hg	25 EST
DC		pKa	NEELY,WB & BLAU,GE (1985)
HL	1.58E-005	atm m ³ /mol	25 EST
OH	1.03E-010	cm ³ /mol sec	25 EST



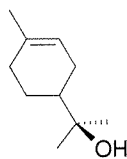
CAS #:		MEVINPHOS	
Formula:		$C_7H_{13}O_6P$	
Mol Weight:		224.15	
MP (deg C):	6.9-21	FP (deg C):	
BP (deg C):	99-103		
BP pressure (mm Hg):		3.00E-001	
Property/Value	Units	Temp	Data Type
WS	6.00E+005	mg/L	EXP
logP	0.13		EXP BENYON,KI ET AL. (1973)
VP	1.30E-004	mm Hg	25 EXP
DC		pKa	WAUCHOPE,RD ET AL. (1991A)
HL	6.39E-011	atm m ³ /mol	25 EST
OH	8.52E-011	cm ³ /mol sec	25 EST



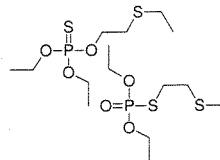
CAS #:		1,1,1-TRICHLOROPROPANE	
Formula:		$C_3H_5Cl_3$	
Mol Weight:		147.43	
MP (deg C):		FP (deg C):	
BP (deg C):	108		
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.90E+003	mg/L	25 EXP
logP	3.17		EST DILLING,WL (1977)
VP	3.16E+001	mm Hg	25 EXP
DC		pKa	MEYLAN,WM & HOWARD,PH (1995)
HL	3.23E-003	atm m ³ /mol	25 EST
OH	2.32E-013	cm ³ /mol sec	25 EST



CAS #:		TERPINEOL	
Formula:		$C_{10}H_{18}O$	
Mol Weight:		154.25	
MP (deg C):		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.98E+003	mg/L	20 EXP
logP	3.33		EST SEIDELL,A (1941)
VP	3.07E-002	mm Hg	25 EST
DC		pKa	MEYLAN,WM & HOWARD,PH (1995)
HL	1.58E-005	atm m ³ /mol	25 EST
OH	1.03E-010	cm ³ /mol sec	25 EST



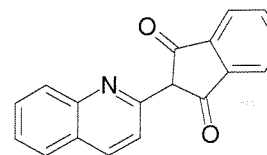
CAS #:		DEMETON	
Formula:		$C_{16}H_{38}O_6P_2S_4$	
Mol Weight:		516.68	
MP (deg C):		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	6.00E+001	mg/L	25 EXP
logP			AUGUSTIJN-BECKERS,PWM ET AL. (1994)
VP	3.00E-004	mm Hg	20 EXP
DC		pKa	AUGUSTIJN-BECKERS,PWM ET AL. (1994)
HL	3.40E-006	atm m ³ /mol	20 EST
OH		cm ³ /mol sec	VP/WSOL

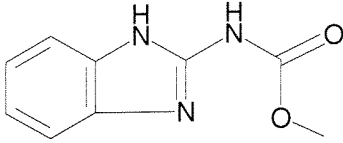


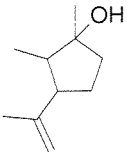
CAS #:		TOXAPHENE	
Formula:			
Mol Weight:			
MP (deg C):		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	5.50E-001	mg/L	20 EXP
logP	4.82		EST MURPHY,TJ ET AL. (1987)
VP	6.69E-006	mm Hg	20 EXP
DC		pKa	LYMAN,WJ ET AL. (1982)
HL	6.00E-006	atm m ³ /mol	20 EXP
OH	2.50E-012	cm ³ /mol sec	25 EST

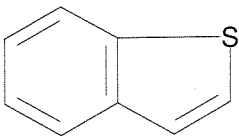
NO STRUCTURE DIAGRAM AVAILABLE

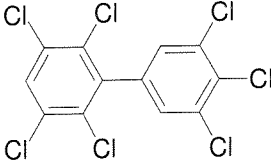
CAS #:		SOLVENT YELLOW 33	
Formula:		$C_{18}H_{11}NO_2$	
Mol Weight:		273.29	
MP (deg C):		FP (deg C):	
BP (deg C):			
BP pressure (mm Hg):			
Property/Value	Units	Temp	Data Type
WS	1.69E-001	mg/L	25 EXP
logP	4.10		EST BAUGHMAN,GL & WEBER,EJ (1991)
VP	9.88E-009	mm Hg	25 EST
DC		pKa	NEELY,WB & BLAU,GE (1985)
HL	6.12E-014	atm m ³ /mol	25 EST
OH	3.58E-011	cm ³ /mol sec	25 EST

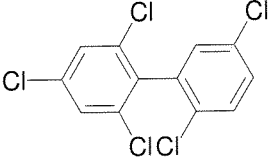


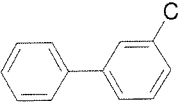
CAS #		010605-21-7		CARBENDAZIM	
Formula:		C ₉ H ₉ N ₃ O ₂			
Mol Weight:		191.19			
MP (deg C):		300 dec		FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	5.80E+000	mg/L	20	EXP	YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP	1.52			EXP	HANSCH,C & LEO,AJ (1985)
VP	4.88E-010	mm Hg	20	EXP	AUGUSTIJN-BECKERS,PWM ET AL. (1994) @ pH=7
DC		pKa			
HL	2.12E-011	atm m ³ /mol	20	EST	VP/WSOL
OH	2.00E-010	cm ³ /mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

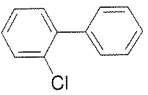
CAS #		011039-70-6		PLINOL	
Formula:		C ₁₀ H ₁₈ O			
Mol Weight:		154.25			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	8.32E+002	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	2.87			EXP	LI,J & PERDUE,EM (1995)
VP	6.22E-002	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	1.34E-005	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	6.66E-011	cm ³ /mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

CAS #		011095-43-5		BENZOTHIOPHENE	
Formula:		C ₈ H ₆ S			
Mol Weight:		134.20			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.92E+002	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	2.99			EST	MEYLAN,WM & HOWARD,PH (1995)
VP	2.39E-001	mm Hg	25	EXT	YAWS,CL (1994B)
DC		pKa			
HL	2.86E-004	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	3.00E-011	cm ³ /mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

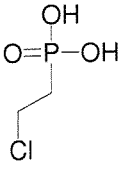
CAS #		011096-82-5		AROCLOR 1260	
Formula:		C ₁₂ H ₃ Cl ₇			
Mol Weight:		395.33			
MP (deg C):				FP (deg C):	
BP (deg C):		385-420			
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.44E-002	mg/L	20	EXP	YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP	6.80			EXP	HANSCH,C ET AL. (1995)
VP	4.05E-005	mm Hg	25	EXP	MABEY,WR ET AL. (1981)
DC		pKa			
HL	3.36E-004	atm m ³ /mol	25	EXP	BURKHARD,LP ET AL. (1985A)
OH		cm ³ /mol sec			

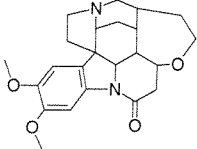
CAS #		011097-69-1		AROCLOR 1254	
Formula:		C ₁₂ H ₅ Cl ₅			
Mol Weight:		326.44			
MP (deg C):				FP (deg C):	
BP (deg C):		365-390			
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	4.30E-002	mg/L	20	EXP	YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP	6.50			EXP	HANSCH,C ET AL. (1995)
VP	7.71E-005	mm Hg	25	EXP	MABEY,WR ET AL. (1981)
DC		pKa			
HL	2.83E-004	atm m ³ /mol	25	EXP	BURKHARD,LP ET AL. (1985A)
OH		cm ³ /mol sec			

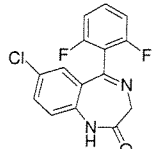
CAS #		011104-28-2		AROCLOR 1221	
Formula:		C ₁₂ H ₉ Cl			
Mol Weight:		188.66			
MP (deg C):				FP (deg C):	
BP (deg C):		275-320			
BP pressure (mm Hg):				51% mono, 32% di, and 11% triphenyl	
Property/Value	Units	Temp	Data Type	Reference	
WS	1.50E+001	mg/L	25	EXP	MABEY,WR ET AL. (1981)
logP	4.70			EXP	HANSCH,C ET AL. (1995)
VP	6.70E-003	mm Hg	25	EXP	MABEY,WR ET AL. (1981)
DC		pKa			
HL	2.28E-004	atm m ³ /mol	25	EXP	BURKHARD,LP ET AL. (1985A)
OH		cm ³ /mol sec			

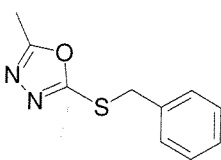
CAS #		011141-16-5		AROCLOR 1232	
Formula:		C ₁₂ H ₉ Cl			
Mol Weight:		188.66			
MP (deg C):		290-325		FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.45E+000	mg/L	25	EXP	MABEY,WR ET AL. (1981)
logP	5.10			EXP	HANSCH,C ET AL. (1995)
VP	4.06E-003	mm Hg	25	EXP	MABEY,WR ET AL. (1981)
DC		pKa			
HL	6.95E-004	atm m ³ /mol	25	EST	VP/WSOL
OH		cm ³ /mol sec			

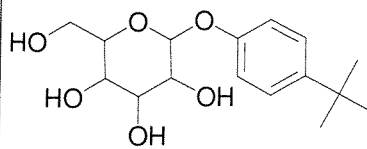
A mixture of isomers:
31% mono, 24% di, and 28% tri

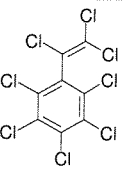
CAS #		011672-87-0		ETHEPHON	
Formula:		C ₂ H ₆ ClO ₃ P			
Mol Weight:		144.50			
MP (deg C):		74-75		FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.00E+006	mg/L		EXP	SHIU,WY ET AL. (1990)
logP	0.05			EST	MEYLAN,WM & HOWARD,PH (1995)
VP	3.78E-005	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	5.70E-012	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	1.05E-012	cm ³ /mol sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

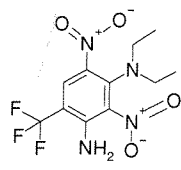
CAS #:		028879-93-8		21,22-DIHYDROBRUCINE	
Formula:		C ₂₃ H ₂₈ N ₂ O ₄			
Mol Weight:		396.49			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	6.17E+002	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	0.84			EXP	HANSCH,C & LEO,AJ (1985)
VP	1.36E-010	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	2.53E-017	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	2.41E-010	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

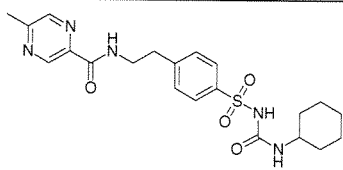
CAS #:		028910-86-3		1,4-BENZODIAZEPIN-2-ONE-5-(26F-PH)7CL	
Formula:		C ₁₅ H ₉ ClF ₂ N ₂ O			
Mol Weight:		306.70			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	5.77E+001	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	2.68			EXP	HANSCH,C & LEO,AJ (1985)
VP	9.35E-009	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	2.42E-010	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	8.72E-012	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

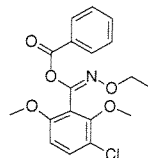
CAS #:		028915-24-4		1,3,4-OXADIAZOLE, 2-METHYL-5-((PHENYLMETHYL)THIO	
Formula:		C ₁₀ H ₁₀ N ₂ O ₅			
Mol Weight:		206.27			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.33E+003	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	1.74			EXP	HANSCH,C ET AL. (1995)
VP	2.30E-005	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	7.44E-009	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	1.63E-011	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

CAS #:		029074-04-2		4-T-BUTYLPHENYL GLUCOPYRANOSIDE	
Formula:		C ₁₆ H ₂₄ O ₆			
Mol Weight:		312.37			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.02E+003	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	1.18			EXP	HANSCH,C & LEO,AJ (1985)
VP	2.70E-012	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	2.97E-015	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	8.83E-011	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

CAS #:		029082-74-4		OCTACHLOROSTYRENE	
Formula:		C ₈ Cl ₈			
Mol Weight:		379.71			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.74E-003	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	7.46			EST	MEYLAN,WM & HOWARD,PH (1995)
VP	1.32E-005	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	2.30E-004	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	1.07E-012	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

CAS #:		029091-05-2		DINITRAMINE	
Formula:		C ₁₁ H ₁₃ F ₃ N ₄ O ₄			
Mol Weight:		322.25			
MP (deg C):		98		FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	1.10E+000	mg/L	25	EXP	YALKOWSKY,SH & DANNENFELSER,RM (1992)
logP	3.96			EST	MEYLAN,WM & HOWARD,PH (1995)
VP	3.60E-006	mm Hg	25	EXP	AUGUSTIJN-BECKERS,PWM ET AL. (1994)
DC		pKa			
HL	1.39E-006	atm m ³ /mol	25	EST	VP/WSOL
OH	1.77E-011	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

CAS #:		029094-61-9		GLIPIZIDE	
Formula:		C ₂₁ H ₂₇ N ₅ O ₄ S			
Mol Weight:		445.54			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	3.72E+001	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	1.91			EXP	HANSCH,C ET AL. (1995)
VP	2.73E-016	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	1.03E-020	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	3.42E-011	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

CAS #:		029104-30-1		BENZOXIMATE	
Formula:		C ₁₈ H ₁₈ ClNO ₅			
Mol Weight:		363.80			
MP (deg C):				FP (deg C):	
BP (deg C):					
BP pressure (mm Hg):					
Property/Value	Units	Temp	Data Type	Reference	
WS	3.33E+000	mg/L	25	EST	MEYLAN,WM ET AL. (1996)
logP	3.73			EXP	SAITO,H ET AL. (1993)
VP	4.40E-008	mm Hg	25	EST	NEELY,WB & BLAU,GE (1985)
DC		pKa			
HL	1.86E-010	atm m ³ /mol	25	EST	MEYLAN,WM & HOWARD,PH (1991)
OH	8.68E-011	cm ³ /molec sec	25	EST	MEYLAN,WM & HOWARD,PH (1993)

ENVIRONMENTAL ORGANIC CHEMISTRY

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A Wiley-Interscience Publication

JOHN WILEY & SONS, INC.

New York / Chichester / Brisbane / Toronto / Singapore

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Library of Congress Cataloging in Publication Data:

Schwarzenbach, René P., 1945-

Environmental organic chemistry / by René P. Schwarzenbach, Philip M. Gschwend, Dieter M. Imboden.

p. cm.

"A Wiley-Interscience Publication."

Includes bibliographical references and index.

ISBN 0-471-83941-8 (cloth)

1. Organic compounds—Environmental aspects. 2. Water chemistry.

I. Gschwend, P. M. II. Imboden, Dieter M., 1943- . III. Title.

TD196.073S39 1992

628.1'68—dc20

92-10737

Printed in the United States of America

10 9 8 7 6 5

compounds for which a LFER of the form:

$$\begin{aligned}\log K_{ow} &= a \log \frac{1}{C_w^{\text{sat}}(1, L)} + b \\ &= -a \log C_w^{\text{sat}}(1, L) + b\end{aligned}\quad (7-14)$$

can be established. In this particular case, one of the organic "solvents" (the pure organic liquid) exhibits special properties; it always forms an ideal mixture with the solute (i.e., $g_s^e = 0$ or $\gamma_s = 1$), and the mole fraction of the solute is equal to 1. Thus, the goodness of the LFER shown in Eq. 7-14 and the values of the regression parameters a and b depend to a great extent on the variability of the activity coefficients in octanol, γ_o , within the set of compounds chosen to establish the LFER, and also, of course, on the accuracy of the experimental data used. Thus, as shown by the examples given in Table 7.2, excellent relationships are found for specific classes of "simple" nonpolar or moderately polar organic compounds, including the alkanes, polycyclic aromatic hydrocarbons, alkylated and halogenated benzenes, and phthalates. Mixing nonpolar with polar compounds and/or with compounds of very different molecular sizes generally results in poorer correlations. This is demonstrated by the substituted benzenes where inclusion of nine additional polar compounds in the set of 23 nonpolar alkyl- and chlorobenzenes substantially decreases the goodness of the fit. Furthermore, as illustrated by the last compound set in Table 7.2, for a very diverse set of chemicals such as the pesticides, very poor correlations may be found. We have already seen that these compounds contain a variety of very different polar groups and, therefore, do not share the same nonideal interactions in octanol. In contrast, a more uniform set of polar compounds like the aliphatic alcohols show much better LFERs. Finally, it should be noted that not all of the scatter in the data found when establishing a relationship between K_{ow} and $C_w^{\text{sat}}(1, L)$ is due to real chemical factors, because experimental errors in both solubility and K_{ow} determina-

TABLE 7.2 Linear Free-Energy Relationships Between Octanol-Water Partition Constants and (Liquid) Aqueous Solubilities for Various Sets of Compounds

Set of Compounds	n	R^2	$\log K_{ow} = -a \log C_w^{\text{sat}}(1, L) + b$	
			$a(\pm \sigma)$	$b(\pm \sigma)$
Alkanes	16	0.91	0.81	-0.20
Polycyclic aromatic hydrocarbons	8	0.99	0.87(± 0.03)	0.68(± 0.16)
Substituted benzenes				
Only nonpolar substituents	23	0.98	0.86(± 0.03)	0.75(± 0.09)
Including polar substituents	32	0.86	0.72(± 0.05)	1.18(± 0.16)
Phthalates	5	1.00	1.06(± 0.03)	-0.22(± 0.09)
PCBs	14	0.92	0.85(± 0.07)	0.78(± 0.47)
Alcohols	41	0.94	0.90	0.83
Miscellaneous pesticides	14	0.81	0.84(± 0.12)	0.12(± 0.49)