

APPENDIX F

CHEMICAL-PHYSICAL PARAMETERS FOR COMPOUNDS NOT INCLUDED IN USEPA'S HHRAP

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A large number of chemical-physical properties are required to calculate environmental concentrations and potential risks for compounds in a combustion source risk assessment. In its 2005 Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities (HHRAP), the U.S. Environmental Protection Agency (USEPA) identified these properties for over 200 compounds. In this risk assessment, there were over 50 additional compounds selected for evaluation, based on the results of the Performance Demonstration Test, for which chemical-physical properties were not provided by HHRAP and which needed to be independently obtained

Table 1, which is included in this appendix, lists the properties compiled for these additional compounds. The methods used to identify these properties were those employed by USEPA for HHRAP, specifically as described in Appendix A-2 of the HHRAP report. In some cases, where data sources recommended in USEPA's Appendix A-2 did not provide information necessary to identify chemical-physical properties, alternative data sources were used. Notes are provided in Table 1 for every chemical-physical parameter indicating the source or basis for each listed value. Table 2 lists the basis for each note included in Table 1.

Either a full set of all chemical-physical properties, or a subset of the properties, was compiled for each compound, depending upon the availability of human health and ecological toxicity criteria. Compounds without chronic human health toxicity criteria and ecological toxicity reference values were not evaluated in the multiple pathway risk assessment and thus, for these compounds, a limited subset of the chemical physical properties was compiled. For these compounds, many of the chemical physical parameters used in USEPA's fate and transport modeling equations to calculate concentrations in plants and animals (e.g., plant, beef, poultry, pork and egg biotransfer coefficients) were not needed and thus were not compiled.

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS
NOT IN USEPA'S HHRAP

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		Molecular weight (g/mole)		Melting point (K)	Melting point (°C)		Vapor pressure (atm) @ 25°C (or 20-30°C)	Vapor pressure (mmHg or Torr) @ 25°C (or 20-30°C)		Solubility in H ₂ O (mg/L) @ 25°C (or 20-30°C)		Henry's law constant (atm-m ³ /mol)		Diffusivity in air (cm ² /sec)		Diffusivity in water (cm ² /sec)		Octanol:water partition coefficient (unitless)	LOG Octanol:water partition coefficient
CAS #	Compound name	MW	Note	Tm		Note	Vp		Note	S	Note	H	Note	Da	Note	Dw	Note	Kow	Log Kow
563-58-6	1,1-Dichloropropene	111	3	183	-90	24	1.19E-01	90.8	3	749	3	0.05	3	0.0823	6a	9.53E-06	6a	3.39E+02	2.53
95-63-6	1,2,4-Trimethylbenzene	120	2	229	-44	2	2.76E-03	2.1	2	57	2	6.16E-03	2	0.0606	6	7.92E-06	6	6.03E+03	3.78
142-28-9	1,3-Dichloropropane	113	3	173.5	-99.5	3	2.39E-02	18.2	3	2750	3	9.76E-04	3	0.074	6	9.87E-06	6	1.00E+02	2
108-60-1	2,2'-oxybis (1-Chloropropane)	171	2	176	-97	2	1.16E-03	0.88	2	1700	2	1.17E-04	2	0.0617	6a	7.14E-06	6a	3.02E+02	2.48
594-20-7	2,2-Dichloropropane	113	2	239.2	-33.8	3	1.78E-01	135	3	391	3	1.61E-02	3	0.072	6	9.48E-06	6	8.32E+02	2.92
625-86-5	2,5-Dimethylfuran	96	3	210.2	-62.8	3	3.41E-02	25.9	3	1470	3	6.55E-03	3	0.0906	6a	1.05E-05	6a	1.74E+02	2.24
2216-30-0	2,5-Dimethylheptane	128	3	194	-79	24	1.25E-02	9.48	3	3.11	3	4	3	0.052	6	6.75E-06	6	4.07E+04	4.61
17559-81-8	2,5-Dione, 3-hexene	112	2	255	-18	24	2.86E-03	2.17	3	3.46E+04	3	1.11E-08	3	0.0818	6a	9.47E-06	6a	3.72E+00	0.57
78-93-3	2-Butanone	72	1	186	-87	1	1.25E-01	95	1	2.20E+05	1	5.60E-05	1	0.0808	6	9.80E-06	6	1.95E+00	0.29
95-49-8	2-Chlorotoluene	127	2	237.4	-35.6	2	4.51E-03	3.43	2	374	2	1.53E-03	2	0.0628	6	8.70E-06	6	2.63E+03	3.42
591-78-6	2-Hexanone	100	2	217.5	-55.5	3	1.53E-02	11.6	2	1.75E+04	2	9.32E-05	3	0.0882	6a	1.02E-05	6a	2.40E+01	1.38
3221-61-2	2-Methyl octane	128	2	192.7	-80.3	3	8.16E-03	6.2	2	2.87	3	5.73	3	0.0597	6	8.24E-06	6	4.90E+04	4.69
91-57-6	2-Methylnaphthalene	140	1	307	34	1	8.95E-05	0.068	1	25	1	5.20E-04	1	0.0522	6	7.75E-06	6	7.94E+03	3.9
34246-54-3	3-Ethyl benzaldehyde	134	24	280.1	7.1	24	1.64E-04	0.125	24	398	24	5.55E-05	24	0.0726	6a	8.40E-06	6a	5.62E+02	2.75

TABLE 1
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		Molecular weight (g/mole)		Melting point (K)	Melting point (oC)		Vapor pressure (atm) @25°C (or 20-30°C)	Vapor pressure (mmHg or Torr) @25°C (or 20-30°C)		Solubility in H2O (mg/L) @25°C (or 20-30°C)		Henry's law constant (atm-m ³ /mol)		Diffusivity in air (cm ² /sec)		Diffusivity in water (cm ² /sec)		Octanol:water partition coefficient (unitless)	LOG Octanol:water partition coefficient
CAS #	Compound name	MW	Note	Tm		Note	Vp		Note	S	Note	H	Note	Da	Note	Dw	Note	Kow	Log Kow
763-93-9	3-Hexen-2-one	98	3	217.5	-55.5	24	1.05E-02	7.96	3	8970	3	5.44E-05	3	0.0894	6a	1.03E-05	6a	2.04E+01	1.31
625-33-2	3-Penten-2-one (ethylidene acetone)	84	2	205	-68	24	5.14E-02	39.1	3	4.62E+04	3	4.10E-05	3	0.0991	6a	1.15E-05	6a	3.31E+00	0.52
141-79-7	3-Penten-2-one, 4-methyl	98	2	214	-59	3	1.45E-02	11	2	2.89E+04	3	3.67E-05	3	0.0734	6	8.83E-06	6	2.34E+01	1.37
534-52-1	4,6-Dinitro-2-methylphenol	198	2	358	85	2	4.26E-07	3.24E-04	2	198	2	4.27E-07	2	0.0276	6	6.91E-06	6	1.32E+02	2.12
106-43-4	4-Chlorotoluene	127	2	280.5	7.5	3	3.54E-03	2.69	2	106	3	4.38E-03	3	0.0625	6	8.65E-06	6	2.14E+03	3.33
4748-78-1	4-Ethyl benzaldehyde	134	24	280.1	7.1	24	1.64E-04	0.125	24	398	24	5.55E-05	24	0.0726	6a	8.40E-06	6a	5.62E+02	2.75
301-02-0	9-Octadecenamide (oleamide)	281	2	432	159	24	4.82E-09	3.66E-06	24	0.046	24	1.26E-06	24	0.0443	6a	5.13E-06	6a	3.02E+06	6.48
208-96-8	Acenaphthylene	150	1	366	93	1	1.20E-06	9.10E-04	1	16	1	1.10E-04	1	0.0449	6	6.98E-06	6	1.26E+04	4.1
7429-90-5	Aluminum	27	1	933	660	1	0.00E+00	0	43	9.50E+04	1	0	3a	0.0772	6	9.57E-06	6	2.14E+00	0.33
92-87-5	Benzidine	180	1	393	120	1	1.05E-11	8.00E-09	1	500	1	3.90E-11	1	0.033	6	1.50E-05	6	5.01E+01	1.7
192-97-2	Benzo(e)pyrene	252	3	450.5	177.5	3	7.50E-12	5.70E-09	3	6.30E-03	3	3.00E-07	3	0.0476	6a	5.51E-06	6a	2.75E+06	6.44
191-24-2	Benzo(g,h,i)perylene	280	1	551	278	2	1.32E-13	1.00E-10	1	2.60E-04	1	3.31E-07	3	0.022	6	5.26E-06	6	3.98E+06	6.6
93-58-3	Benzoic acid, methyl ester (methyl benzoate)	136	2	258	-15	3	5.00E-04	0.38	3	2100	3	3.24E-05	3	0.0577	6	8.39E-06	6	1.32E+02	2.12
111-91-1	Bis(2-chloroethoxy) methane	173	2	241	-32	2	1.84E-07	1.40E-04	2	121000	2	1.70E-07	2	0.044	6	8.46E-06	6	5.62E+00	0.75

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CAS #	Compound name	MW	Note	Tm		Note	Vp		Note	S	Note	H	Note	Da	Note	Dw	Note	Kow	Log Kow
108-86-1	Bromobenzene	157	2	242.4	-30.6	3	5.50E-03	4.18	3	446	2	2.47E-03	3	0.0537	6	9.30E-06	6	9.77E+02	2.99
74-97-5	Bromochloromethane	129	2	185.1	-87.9	3	1.88E-01	142.5	2	1.67E+04	3	1.46E-03	3	0.0688	6	1.00E-05	6	2.57E+01	1.41
104-51-8	Butylbenzene, n-	134	2	185.1	-87.9	3	1.39E-03	1.06	3	11.8	3	1.59E-02	3	0.057	6	8.12E-06	6	2.40E+04	4.38
135-98-8	Butylbenzene, sec	134	3	190.3	-82.7	3	2.30E-03	1.75	3	17.6	3	1.76E-02	3	0.057	6	8.12E-06	6	3.72E+04	4.57
98-06-6	Butylbenzene, tert	134	2	215.2	-57.8	3	2.89E-03	2.2	3	29.5	3	1.32E-02	3	0.0565	6	8.02E-06	6	1.29E+04	4.11
86-74-8	Carbazole	170	1	523	250	1	9.21E-07	7.00E-04	1	1.2	1	8.70E-08	1	3.90E-02	5	7.03E-06	5	5.01E+03	3.7
7440-48-4	Cobalt	59	1	1773	1500	1	0.00E+00	0	43	8.70E+04	24	0	3a	0.0772	6	9.57E-06	6	1.70E+00	0.23
7440-50-8	Copper	64	1	1373	1100	1	5.58E-12	4.24E-09	3	4.21E+05	3	2.50E-02	1	0.0772	6	9.57E-06	6	2.69E-01	-0.57
2303-16-4	Diallate	270	2	300.5	27.5	2	1.97E-07	1.50E-04	2	14	2	3.80E-06	2	0.0213	6	5.27E-06	6	6.31E+04	4.8
132-64-9	Dibenzofuran	170	1	360	87	1	2.37E-07	1.80E-04	1	3.1	1	1.30E-05	1	0.0238	6	6.00E-06	6	1.26E+04	4.1
122-39-4	Diphenylamine	159	2	326.5	53.5	2	8.79E-07	6.68E-04	2	35.7	2	4.96E-07	2	0.058	6	6.31E-06	6	3.16E+03	3.5
1031-07-8	Endosulfan sulfate	423	3	454.5	181.5	3	3.68E-10	2.80E-07	3	0.48	3	3.25E-07	3	0.0182	6	4.45E-06	6	4.57E+03	3.66
7421-93-4	Endrin aldehyde	380	1	420	147	8	2.63E-10	2.00E-07	1	2.40E-02	1	4.20E-06	1	0.019	6	4.37E-06	6	6.31E+04	4.8
53494-70-5	Endrin ketone	381	3	419	146	24	1.21E-07	9.20E-05	24	0.222	3	2.02E-08	3	0.0362	6a	4.19E-06	6a	9.77E+04	4.99

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CAS #	Compound name	MW	Note	Tm		Note	Vp		Note	S	Note	H	Note	Da	Note	Dw	Note	Kow	Log Kow
76-13-1	Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane)	187	2	236.6	-36.4	2	4.36E-01	331.6	2	170	2	4.81E-01	2	0.078	6	8.20E-06	6	1.45E+03	3.16
74-88-4	Iodomethane	142	2	206.6	-66.4	2	5.32E-01	404.46	2	13848	2	5.26E-03	2	0.0524	6	7.76E-06	6	3.24E+01	1.51
99-87-6	Isopropyl toluene, p-	134	2	204.1	-68.9	3	1.92E-03	1.46	2	23.4	2	1.10E-02	2	0.056	6	7.33E-06	6	1.26E+04	4.1
7439-96-5	Manganese	55	1	1473	1200	1	5.58E-12	4.24E-09	3	1100	1	0.0245	3	0.0772	6	9.57E-06	6	1.70E+00	0.23
62-75-9	N-nitrosodimethylamine	74	2	223	-50	2	3.55E-03	2.7	2	1.00E+06	8	1.20E-06	2	0.104	6	1.00E-05	6	2.69E-01	-0.57
198-55-0	Perylene	252	3	547	274	3	6.91E-12	5.25E-09	3	0.0004	3	3.65E-06	3	0.0223	6	5.56E-06	6	1.78E+06	6.25
2240-47-3	Phosphine imide, P,P,P-triphenyl	277	24	417	144	24	6.29E-09	4.78E-06	24	0.755	24	1.43E-07	24	0.0447	6a	5.18E-06	6a	1.20E+05	5.08
103-65-1	Propylbenzene, n-	120	2	173.5	-99.5	3	4.50E-03	3.42	2	52.2	2	1.05E-02	2	0.0601	6	7.83E-06	6	3.72E+03	3.57
7440-62-2	Vanadium	51	1	2173	1900	1	0.00E+00	0	43	700	1	0	3a	0.0772	6	9.57E-06	6	1.70E+00	0.23
58-89-9	γ-BHC (Lindane)	290	1	383	110	1	5.39E-07	4.10E-04	1	7.3	1	1.40E-05	2	1.42E-02	5	7.34E-06	5	3.98E+03	3.6
319-86-8	δ-BHC	291	2	415	142	2	4.63E-08	3.52E-05	2	31.4	2	4.29E-07	2	0.0221	6	5.57E-06	6	1.38E+04	4.14
110-54-3	1-Hexane (n-hexane)	86	2	177.7	-95.3	3	1.99E-01	151.3	2	124	2	1.8	3	0.2	6	7.77E-06	6	7.94E+03	3.9
79-10-7	Acrylic Acid	72	2	286.5	13.5	2	5.26E-03	4	2	1.00E+06	8	1.17E-07	2	0.098	6	1.06E-05	6	1.45E+00	0.161
107-21-1	Ethylene Glycol	62	2	260.4	-12.6	2	1.21E-04	0.092	2	1.00E+06	8	6.00E-08	2	0.108	6	1.22E-05	6	4.37E-02	-1.36
80-62-6	Methyl methacrylate	100	2	225	-48	3	5.05E-02	38.4	2	1.50E+04	2	3.37E-04	2	0.077	6	8.60E-06	6	2.40E+01	1.38

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CAS #	Compound name	MW	Note	Tm		Note	Vp		Note	S	Note	H	Note	Da	Note	Dw	Note	Kow	Log Kow
1634-04-4	methyl tert-butyl ether	88	1	163	-110	1	3.29E-01	250	1	5.10E+04	1	5.90E-04	1	0.086	6	1.01E-05	6	1.58E+01	1.2
75-56-9	Propylene oxide	58	2	161	-112	2	7.08E-01	538	2	590000	2	1.23E-04	2	0.104	6	1.00E-05	6	1.07E+00	0.03
33213-65-9	Endosulfan II	407	1	382	109	2	1.3158E-08	1.00E-05	1	0.45	2	1.30E-05	1	0.0346	6a	4.01E-06	6a	6.31E+03	3.8
7446-09-5	Sulfur dioxide	64	3	201	-72	3	3.94868421	3.00E+03	2	1.07E+05	3	8.10E-04	3	0.1188	6a	1.38E-05	6a	6.31E-03	-2.2
10102-44-0	Nitrogen dioxide	46	3	263.7	-9.3	3	1.19460526	9.08E+02	2	1.71E+05	3	2.45E-02	3	0.1480	6a	1.71E-05	6a	2.63E-01	-0.58
Compounds evaluated for fugitive vapor emissions only																			
106-99-0	1,3-Butadiene	54.09	3	164	-109	2	2.77236842	2.11E+03	2	7.35E+02	2	7.36E-02	2	0.1328	6a	1.54E-05	6a	9.77E+01	1.99
110-82-7	Cyclohexane	84.16	3	279.5	6.5	2	0.12736842	9.68E+01	2	5.50E+01	2	1.95E-01	2	0.0989	6a	1.15E-05	6a	2.75E+03	3.44

-- = Not applicable - compound did not have chronic human health toxicity data, or ecological risk assessment toxicity reference values (TRVs), and thus was not evaluated in the multiple pathway fate and transport modeling.

NA = Not applicable. Compound was only evaluated for the inhalation pathway in the human health risk assessment addressing potential fugitive emissions.

TABLE 1
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			Soil organic carbon:water partition coefficient (mL H2O/ g soil)	LOG Soil organic carbon:water partition coefficient (Koc) (mL H2O/ g soil)		Soil-water partition coefficient (mL H2O/g soil OR cm3 H2O/g soil)		Suspended sediment-surface water partition coefficient (L H2O/kg suspended sed OR cm3 H2O/g suspended sed)		Bed sediment-pore water partition coefficient (L H2O/kg bottom sed OR cm3 H2O/g bottom sed)		Soil loss constant due to biotic and abiotic degradation (yr-1)		Fraction of air concentration in vapor phase (unitless)	Liquid phase vapor pressure (atm) (used only for compounds that are solids at ambient T)	Root concentration factor (g COPC/g DW plant) / (g COPC/mL soil water)	
CAS #	Compound name	Note	Koc	Log Koc	Note	Kd,s	Note	Kd,sw	Note	Kd,bs	Note	Ksg	Note	fv	Vp	Note	RCF DW
563-58-6	1,1-Dichloropropene	3			--		--		--		--	0	44	1.0		16	
95-63-6	1,2,4-Trimethylbenzene	2	1.18E+03	3.0718	10	1.18E+01	13	8.85E+01	14	4.72E+01	15	0	44	1.0		16	1.89E+02
142-28-9	1,3-Dichloropropane	3	9.25E+01	1.9663	9	9.25E-01	13	6.94E+00	14	3.70E+00	15	0	44	1.0		16	8.05E+00
108-60-1	2,2'-oxybis (1-Chloropropane)	2	57		2	5.70E-01	13	4.28E+00	14	2.28E+00	15	0	44	1.0		16	1.89E+01
594-20-7	2,2-Dichloropropane	3	2.46E+02	2.3907	10	2.46E+00	13	1.84E+01	14	9.84E+00	15	0	44	1.0		16	4.12E+01
625-86-5	2,5-Dimethylfuran	3	7.12E+01	1.8523	10	7.12E-01	13	5.34E+00	14	2.85E+00	15	0	44	1.0		16	1.23E+01
2216-30-0	2,5-Dimethylheptane	3	0		--		--		--		--	0	44	1.0		16	
17559-81-8	2,5-Dione, 3-hexene	3	0		--		--		--		--	0	44	1.0		16	
78-93-3	2-Butanone	1	1.93E+00	0.2854	9	0.29	1	1.45E-01	14	7.72E-02	15	0	44	1.0		16	6.70E+00
95-49-8	2-Chlorotoluene	2	550		2	5.50E+00	13	4.13E+01	14	2.20E+01	15	0	44	1.0		16	9.99E+01
591-78-6	2-Hexanone	2	2.27E+01	1.3568	9	2.27E-01	13	1.71E+00	14	9.10E-01	15	0	44	1.0		16	8.99E+00
3221-61-2	2-Methyl octane	3			--		--		--		--	0	44	1.0		16	
91-57-6	2-Methylnaphthalene	1	6.82E+03	3.8340	9	950	1	5.12E+02	14	2.73E+02	15	0	44	1.000E+00	1.10E-04	17,16	2.34E+02
34246-54-3	3-Ethyl benzaldehyde	24	102.2		24		--		--		--	0	44	1.0		16	

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

			Soil organic carbon:water partition coefficient (mL H2O/ g soil)	LOG Soil organic carbon:water partition coefficient (Koc) (mL H2O/ g soil)		Soil-water partition coefficient (mL H2O/g soil OR cm3 H2O/g soil)		Suspended sediment-surface water partition coefficient (L H2O/kg suspended sed OR cm3 H2O/g suspended sed)		Bed sediment-pore water partition coefficient (L H2O/kg bottom sed OR cm3 H2O/g bottom sed)		Soil loss constant due to biotic and abiotic degradation (yr-1)		Fraction of air concentration in vapor phase (unitless)	Liquid phase vapor pressure (atm) (used only for compounds that are solids at ambient T)	Root concentration factor (g COPC/g DW plant) / (g COPC/mL soil water)	
CAS #	Compound name	Note	Koc	Log Koc	Note	Kd,s	Note	Kd,sw	Note	Kd,bs	Note	Ksg	Note	fv	Vp	Note	RCF DW
763-93-9	3-Hexen-2-one	3			--		--		--		--	0	44	1.0		16	
625-33-2	3-Penten-2-one (ethylidene acetone)	3			--		--		--		--	0	44	1.0		16	
141-79-7	3-Penten-2-one, 4-methyl	3			--		--		--		--	0	44	1.0		16	
534-52-1	4,6-Dinitro-2-methylphenol	2	257		2	2.57E+00	13	1.93E+01	14	1.03E+01	15	0	44	9.996E-01	1.67E-06	17,16	9.96E+00
106-43-4	4-Chlorotoluene	3	5.19E+02	2.7154	10	5.19E+00	13	3.89E+01	14	2.08E+01	15	0	44	1.0		16	8.51E+01
4748-78-1	4-Ethyl benzaldehyde	24	102.2		24		--		--		--	0	44	1.0		16	
301-02-0	9-Octadecenamide (oleamide)	24	1.02E+05		24		--		--		--	0	44	9.942E-01	1.02E-07	17,16	
208-96-8	Acenaphthylene	1	1.07E+04	4.0306	9	1.50E+03	1	8.05E+02	14	4.29E+02	15	0	44	9.999E-01	5.64E-06	17,16	3.33E+02
7429-90-5	Aluminum	24	0		43	9.9	1	9.9	14b	9.9	14b	0	44	0		16a	0
92-87-5	Benzidine	1	4.69E+01	1.6714	9	6.5	1	3.52E+00	14	1.88E+00	15	0.13	45	1.335E-01	9.17E-11	17,16	1.10E+01
192-97-2	Benzo(e)pyrene	3			--		--		--		--	0	44	2.893E-01	2.42E-10	17,16	
191-24-2	Benzo(g,h,i)perylene	1	3.08E+06	6.4881	9	4.50E+05	1	2.31E+05	14	1.23E+05	15	0	44	6.586E-02	4.20E-11	17,16	2.81E+04
93-58-3	Benzoic acid, methyl ester (methyl benzoate)	3	1.21E+02	2.0842	9	1.21E+00	13	9.11E+00	14	4.86E+00	15	0	44	1.0		16	9.96E+00
111-91-1	Bis(2-chloroethoxy) methane	2	61		2	6.10E-01	13	4.58E+00	14	2.44E+00	15	0	44	1.0		16	7.19E+00

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

			Soil organic carbon:water partition coefficient (mL H2O/ g soil)	LOG Soil organic carbon:water partition coefficient (Koc) (mL H2O/ g soil)		Soil-water partition coefficient (mL H2O/g soil OR cm3 H2O/g soil)		Suspended sediment-surface water partition coefficient (L H2O/kg suspended sed OR cm3 H2O/g suspended sed)		Bed sediment-pore water partition coefficient (L H2O/kg bottom sed OR cm3 H2O/g bottom sed)		Soil loss constant due to biotic and abiotic degradation (yr-1)		Fraction of air concentration in vapor phase (unitless)	Liquid phase vapor pressure (atm) (used only for compounds that are solids at ambient T)		Root concentration factor (g COPC/g DW plant) / (g COPC/mL soil water)
CAS #	Compound name	Note	Koc	Log Koc	Note	Kd,s	Note	Kd,sw	Note	Kd,bs	Note	Ksg	Note	fv	Vp	Note	RCF DW
108-86-1	Bromobenzene	2	151		2	1.51E+00	13	1.13E+01	14	6.04E+00	15	0	44	1.0		16	4.66E+01
74-97-5	Bromochloromethane	3			--		--		--		--	0	44	1.0		16	
104-51-8	Butylbenzene, n-	3	2512		2		--		--		--	0	44	1.0		16	
135-98-8	Butylbenzene, sec	3	4.98E+03	3.6974	10		--		--		--	0	44	1.0		16	
98-06-6	Butylbenzene, tert	3	2.15E+03	3.3331	10	2.15E+01	13	1.61E+02	14	8.61E+01	15	0	44	1.0		16	3.39E+02
86-74-8	Carbazole	1	3390		5	520	1	2.54E+02	14	1.36E+02	15	0	44	1.000E+00	1.55E-04	17,16	1.64E+02
7440-48-4	Cobalt	1	0		43	45	1	45	14b	45	14b	0	44	0		16a	0
7440-50-8	Copper	1	0		43	430	1	430	14b	430	14b	0	44	0		16a	0
2303-16-4	Diallate	2	273		2		--		--		--	0	44	9.972E-01	2.09E-07	17,16	
132-64-9	Dibenzofuran	1	1.07E+04	4.0306	9	1700	1	8.05E+02	14	4.29E+02	15	0	44	9.994E-01	9.73E-07	17,16	3.33E+02
122-39-4	Diphenylamine	2	600		2	347	2	4.50E+01	14	2.40E+01	15	0	44	9.996E-01	1.68E-06	17,16	1.15E+02
1031-07-8	Endosulfan sulfate	3	3.96E+03	3.5981	9	3.96E+01	13	2.97E+02	14	1.59E+02	15	0	44	9.563E-01	1.30E-08	17,16	1.53E+02
7421-93-4	Endrin aldehyde	1	2.00E+04	4.3	8	8000	1	1.50E+03	14	7.98E+02	15	0	44	8.770E-01	4.24E-09	17,16	1.15E+03
53494-70-5	Endrin ketone	3			--		--		--		--	0	44	9.997E-01	1.91E-06	17,16	

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

			Soil organic carbon:water partition coefficient (mL H2O/ g soil)	LOG Soil organic carbon:water partition coefficient (Koc) (mL H2O/ g soil)		Soil-water partition coefficient (mL H2O/g soil OR cm3 H2O/g soil)		Suspended sediment-surface water partition coefficient (L H2O/kg suspended sed OR cm3 H2O/g suspended sed)		Bed sediment-pore water partition coefficient (L H2O/kg bottom sed OR cm3 H2O/g bottom sed)		Soil loss constant due to biotic and abiotic degradation (yr-1)		Fraction of air concentration in vapor phase (unitless)	Liquid phase vapor pressure (atm) (used only for compounds that are solids at ambient T)	Root concentration factor (g COPC/g DW plant) / (g COPC/mL soil water)	
CAS #	Compound name	Note	Koc	Log Koc	Note	Kd,s	Note	Kd,sw	Note	Kd,bs	Note	Ksg	Note	fv	Vp	Note	RCF DW
76-13-1	Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane)	2	372		2	3.72E+00	13	2.79E+01	14	1.49E+01	15	0	44	1.0		16	6.30E+01
74-88-4	Iodomethane	2	158		2	1.58E+00	13	1.19E+01	14	6.32E+00	15	0	44	1.0		16	9.69E+00
99-87-6	Isopropyl toluene, p-	2	2.11E+03	3.3252	10	2.11E+01	13	1.59E+02	14	8.46E+01	15	0	44	1.0		16	3.33E+02
7439-96-5	Manganese	1	0		43	65	1	65	14b	65	14b	0	44	0		16a	0
62-75-9	N-nitrosodimethylamine	2	12		2	1.20E-01	13	9.00E-01	14	4.80E-01	15	0	44	1.0		16	6.39
198-55-0	Perylene	3	8.03E+05		24		--		--		--	0	44	7.716E-01	2.01E-09	17,16	
2240-47-3	Phosphine imide, P,P,P-triphenyl	24	6.96E+05		24		--		--		--	0	44	9.938E-01	9.47E-08	17,16	
103-65-1	Propylbenzene, n-	2	741		2		--		--		--	0	44	1.0		16	
7440-62-2	Vanadium	24	0		43	1000	1	1000	14b	1000	14b	0	44	0		16a	0
58-89-9	γ-BHC (Lindane)	1	1352		5	2.1	1	101.4	14	5.41E+01	15	0	44	9.998E-01	3.74E-06	17,16	1.37E+02
319-86-8	δ-BHC	2	4260		2	4.26E+01	13	3.20E+02	14	1.70E+02	15	0	44	9.991E-01	6.66E-07	17,16	3.58E+02
110-54-3	1-Hexane (n-hexane)	3	1.47E+03	3.1668	10	1.47E+01	13	1.10E+02	14	5.87E+01	15	0	44	1.0		16	2.34E+02
79-10-7	Acrylic Acid	2	1.45E-02	-1.84	12	1.45E-04	13	1.08E-03	14	5.78E-04	15	0	44	1.0		16	6.62E+00
107-21-1	Ethylene Glycol	2	4		2	4.00E-02	13	3.00E-01	14	1.60E-01	15	0	44	1.0		16	6.39
80-62-6	Methyl methacrylate	2	22		2	2.20E-01	13	1.65E+00	14	8.80E-01	15	0	44	1.0		16	8.99E+00

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

			Soil organic carbon:water partition coefficient (mL H2O/ g soil)	LOG Soil organic carbon:water partition coefficient (Koc) (mL H2O/ g soil)		Soil-water partition coefficient (mL H2O/g soil OR cm3 H2O/g soil)		Suspended sediment-surface water partition coefficient (L H2O/kg suspended sed OR cm3 H2O/g suspended sed)		Bed sediment- pore water partition coefficient (L H2O/kg bottom sed OR cm3 H2O/g bottom sed)		Soil loss constant due to biotic and abiotic degradation (yr- 1)		Fraction of air concentration in vapor phase (unitless)	Liquid phase vapor pressure (atm) (used only for compounds that are solids at ambient T)	Root concentration factor (g COPC/g DW plant) / (g COPC/mL soil water)	
CAS #	Compound name	Note	Koc	Log Koc	Note	Kd,s	Note	Kd,sw	Note	Kd,bs	Note	Ksg	Note	fv	Vp	Note	RCF DW
1634-04-4	methyl tert-butyl ether	1	1.51E+01	1.1799	9	8.9	1	1.13E+00	14	6.05E-01	15	0	44	1.0		16	8.26E+00
75-56-9	Propylene oxide	2	25		2	2.50E-01	13	1.88E+00	14	1.00E+00	15	0	44	1.0		16	6.55E+00
33213-65-9	Endosulfan II	1	6770		2	4.3	1	5.08E+02	14	2.71E+02	15	0	44	9.934E-01	8.92E-08	17,16	1.96E+02
7446-09-5	Sulfur dioxide	3	2.99		24	2.99E-02	13	2.24E-01	14	1.20E-01	15	0	44	1.0		16	6.31E+00
10102-44-0	Nitrogen dioxide	3	5.54		24	5.54E-02	13	4.16E-01	14	2.22E-01	15	0	44	1.0		16	6.39E+00
Compounds evaluated for fugitive vap																	
106-99-0	1,3-Butadiene	2	116		2	NA		NA		NA		NA		1.0		16	NA
110-82-7	Cyclohexane	2	482		2	NA		NA		NA		NA		1.0		16	NA

-- = Not applicable - compound did not have chronic human health toxicity data, or ecological risk assessment toxicity reference values (TRVs), and thus was not evaluated in the multiple pathway fate and transport modeling.

NA = Not applicable. Compound was only evaluated for the inhalation pathway in the human health risk assessment addressing potential fugitive emissions.

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		RCF in fresh wt (FW) (g COPC/g FW plant) / (g COPC/mL soil water)		Plant-soil bioconcentration factor for below ground produce (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for aboveground produce (HHRAP variable = Br_{ag}) (same value used for Br_{grain}) (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for forage and silage (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Air-to-plant biotransfer factor in aboveground produce (HHRAP variable = Bv_{ag}) (g COPC/g DW plant)/ (g COPC/g air) (unitless)		LOG Bvol		Air-to-plant biotransfer factor in forage and silage (g COPC/g DW plant)/ (g COPC/g air) (unitless)	
CAS #	Compound name	RCF FW	Note	Br, root-veg	Note	Br, leafy-veg	Note	Br, forage	Note	Bv, leafy veg		Log Bvol	Note	Bv, forage	Note
563-58-6	1,1-Dichloropropene		--		--	0	--		--				--		--
95-63-6	1,2,4-Trimethylbenzene	2.46E+01	18,20	1.60E+01	22	2.53E-01	25	2.53E-01	25	9.62E-02		2.97E+00	28	9.62E-02	28
142-28-9	1,3-Dichloropropane	1.05E+00	18,20	8.71E+00	22	2.70E+00	25	2.70E+00	25	7.72E-03		1.87E+00	28	7.72E-03	28
108-60-1	2,2'-oxybis (1-Chloropropane)	2.45E+00	18,20	3.31E+01	22	1.43E+00	25	1.43E+00	25	2.09E-01		3.31E+00	28	2.09E-01	28
594-20-7	2,2-Dichloropropane	5.35E+00	18,20	1.67E+01	22	7.95E-01	25	7.95E-01	25	4.47E-03		1.64E+00	28	4.47E-03	28
625-86-5	2,5-Dimethylfuran	1.60E+00	18,20	1.73E+01	22	1.96E+00	25	1.96E+00	25	2.07E-03		1.30E+00	28	2.07E-03	28
2216-30-0	2,5-Dimethylheptane		--		--		--		--	0			--		--
17559-81-8	2,5-Dione, 3-hexene		--		--		--		--	0			--		--
78-93-3	2-Butanone	8.71E-01	19,20	2.31E+01	22	8.38	25a	8.38	25a	2.03E-03		1.29E+00	28	2.03E-03	28
95-49-8	2-Chlorotoluene	1.30E+01	18,20	1.82E+01	22	4.09E-01	25	4.09E-01	25	1.60E-01		3.19E+00	28	1.60E-01	28
591-78-6	2-Hexanone	1.17E+00	19,20	3.95E+01	22	6.17E+00	25	6.17E+00	25	1.77E-02		2.23E+00	28	1.77E-02	28
3221-61-2	2-Methyl octane		--		--		--	0	--				--		--
91-57-6	2-Methylnaphthalene	3.04E+01	18,20	2.46E-01	22	2.16E-01	25	2.16E-01	25	1.53E+00		4.17E+00	28	1.53E+00	28
34246-54-3	3-Ethyl benzaldehyde		--		--		--	0	--				--		--

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		RCF in fresh wt (FW) (g COPC/g FW plant) / (g COPC/mL soil water)		Plant-soil bioconcentration factor for below ground produce (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for aboveground produce (HHRAP variable = Br_{ag}) (same value used for Br_{grain}) (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for forage and silage (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Air-to-plant biotransfer factor in aboveground produce (HHRAP variable = Bv_{ag}) (g COPC/g DW plant)/ (g COPC/g air) (unitless)		LOG Bvol		Air-to-plant biotransfer factor in forage and silage (g COPC/g DW plant)/ (g COPC/g air) (unitless)	
CAS #	Compound name	RCF FW	Note	Br, root-veg	Note	Br, leafy-veg	Note	Br, forage	Note	Bv, leafy veg		Log Bvol	Note	Bv, forage	Note
763-93-9	3-Hexen-2-one		--		--		--	0	--				--		--
625-33-2	3-Penten-2-one (ethylidene acetone)		--		--		--	0	--				--		--
141-79-7	3-Penten-2-one, 4-methyl		--		--		--		--				--		--
534-52-1	4,6-Dinitro-2-methylphenol	1.30E+00	18,20	3.88E+00	22	2.30E+00	25	2.30E+00	25	2.37E+01		5.36E+00	28	2.37E+01	28
106-43-4	4-Chlorotoluene	1.11E+01	18,20	1.64E+01	22	4.61E-01	25	4.61E-01	25	4.49E-02		2.64E+00	28	4.49E-02	28
4748-78-1	4-Ethyl benzaldehyde		--		--		--		--				--		--
301-02-0	9-Octadecenamide (oleamide)		--		--		--		--				--		--
208-96-8	Acenaphthylene	4.34E+01	18,20	2.22E-01	22	1.65E-01	25	1.65E-01	25	1.18E+01		5.06E+00	28	1.18E+01	28
7429-90-5	Aluminum		21a	6.50E-04	23	0.0011	27	1	26	0			29	0	29
92-87-5	Benzidine	1.44E+00	19,20	1.70E+00	22	4.03E+00	25	4.03E+00	25	9.26E+04		8.95E+00	28	9.26E+04	28
192-97-2	Benzo(e)pyrene		--		--		--	0	--				--		--
191-24-2	Benzo(g,h,i)perylene	3.65E+03	18,20	6.24E-02	22	5.93E-03	25	5.93E-03	25	1.80E+06		1.02E+01	28	1.80E+06	28
93-58-3	Benzoic acid, methyl ester (methyl benzoate)	1.30E+00	18,20	8.21E+00	22	2.30E+00	25	2.30E+00	25	3.12E-01		3.48E+00	28	3.12E-01	28
111-91-1	Bis(2-chloroethoxy) methane	9.34E-01	19,20	1.18E+01	22	8.38	25a	8.38	25a	2.07E+00		4.30E+00	28	2.07E+00	28

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		RCF in fresh wt (FW) (g COPC/g FW plant) / (g COPC/mL soil water)		Plant-soil bioconcentration factor for below ground produce (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for aboveground produce (HHRAP variable = Br_{ag}) (same value used for Br_{grain}) (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for forage and silage (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Air-to-plant biotransfer factor in aboveground produce (HHRAP variable = Bv_{ag}) (g COPC/g DW plant) / (g COPC/g air) (unitless)		LOG Bvol		Air-to-plant biotransfer factor in forage and silage (g COPC/g DW plant) / (g COPC/g air) (unitless)	
CAS #	Compound name	RCF FW	Note	Br, root-veg	Note	Br, leafy-veg	Note	Br, forage	Note	Bv, leafy veg		Log Bvol	Note	Bv, forage	Note
108-86-1	Bromobenzene	6.06E+00	18,20	3.09E+01	22	7.24E-01	25	7.24E-01	25	3.46E-02		2.53E+00	28	3.46E-02	28
74-97-5	Bromochloromethane		--		--		--	0	--	0			--		--
104-51-8	Butylbenzene, n-		--		--		--	0	--	0			--		--
135-98-8	Butylbenzene, sec		--		--		--		--				--		--
98-06-6	Butylbenzene, tert	4.41E+01	18,20	1.58E+01	22	1.63E-01	25	1.63E-01	25	1.01E-01		2.99E+00	28	1.01E-01	28
86-74-8	Carbazole	2.13E+01	18,20	3.16E-01	22	2.81E-01	25	2.81E-01	25	5.60E+03		7.74E+00	28	5.60E+03	28
7440-48-4	Cobalt		21a	7.00E-03	23	0.0086	27	0.02	26	0			29	0	29
7440-50-8	Copper		21a	0.25	23	0.27	27	0.4	26	0			29	0	29
2303-16-4	Diallylate		--		--		--		--				--		--
132-64-9	Dibenzofuran	4.34E+01	18,20	1.96E-01	22	1.65E-01	25	1.65E-01	25	9.99E+01		5.99E+00	28	9.99E+01	28
122-39-4	Diphenylamine	1.50E+01	18,20	3.32E-01	22	3.67E-01	25	3.67E-01	25	6.01E+02		6.77E+00	28	6.01E+02	28
1031-07-8	Endosulfan sulfate	1.99E+01	18,20	3.86E+00	22	2.97E-01	25	2.97E-01	25	1.36E+03		7.12E+00	28	1.36E+03	28
7421-93-4	Endrin aldehyde	1.50E+02	18,20	1.44E-01	22	6.51E-02	25	6.51E-02	25	1.72E+03		7.22E+00	28	1.72E+03	28
53494-70-5	Endrin ketone		--		--		--		--				--		--

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		RCF in fresh wt (FW) (g COPC/g FW plant) / (g COPC/mL soil water)		Plant-soil bioconcentration factor for below ground produce (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for aboveground produce (HHRAP variable = Br_{ag}) (same value used for Br_{grain}) (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for forage and silage (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Air-to-plant biotransfer factor in aboveground produce (HHRAP variable = Bv_{ag}) (g COPC/g DW plant)/ (g COPC/g air) (unitless)		LOG Bvol		Air-to-plant biotransfer factor in forage and silage (g COPC/g DW plant)/ (g COPC/g air) (unitless)	
CAS #	Compound name	RCF FW	Note	Br, root-veg	Note	Br, leafy-veg	Note	Br, forage	Note	Bv, leafy veg		Log Bvol	Note	Bv, forage	Note
76-13-1	Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane)	8.19E+00	18,20	1.69E+01	22	5.77E-01	25	5.77E-01	25	2.69E-04		4.17E-01	28	2.69E-04	28
74-88-4	Iodomethane	1.26E+00	19,20	6.13E+00	22	5.19E+00	25	5.19E+00	25	4.31E-04		6.21E-01	28	4.31E-04	28
99-87-6	Isopropyl toluene, p-	4.34E+01	18,20	1.58E+01	22	1.65E-01	25	1.65E-01	25	1.18E-01		3.06E+00	28	1.18E-01	28
7439-96-5	Manganese		21a	0.05	23	0.075	27	0.25	26	0			29	0	29
62-75-9	N-nitrosodimethylamine		21	5.33E+01	22	8.38	25a	8.38	25a	1.15E-02		2.05E+00	28	1.15E-02	28
198-55-0	Perylene		--		--		--		--				--		--
2240-47-3	Phosphine imide, P,P,P-triphenyl		--		--		--		--	0			--		--
103-65-1	Propylbenzene, n-		--		--		--		--	0			--		--
7440-62-2	Vanadium		21a	3.00E-03	23	0.0033	27	5.50E-03	26	0			29	0	29
58-89-9	γ-BHC (Lindane)	1.79E+01	18,20	6.54E+01	22	3.22E-01	25	3.22E-01	25	2.72E+01		5.42E+00	28	2.72E+01	28
319-86-8	δ-BHC	4.65E+01	18,20	8.40E+00	22	1.57E-01	25	1.57E-01	25	3.34E+03		7.51E+00	28	3.34E+03	28
110-54-3	1-Hexane (n-hexane)	3.04E+01	18,20	1.59E+01	22	2.16E-01	25	2.16E-01	25	4.42E-04		6.32E-01	28	4.42E-04	28
79-10-7	Acrylic Acid	8.60E-01	19,20	4.58E+04	22	8.38	25a	8.38	25a	7.08E-01		3.84E+00	28	7.08E-01	28
107-21-1	Ethylene Glycol		21	1.60E+02	22	8.38	25a	8.38	25a	3.31E-02		2.51E+00	28	3.31E-02	28
80-62-6	Methyl methacrylate	1.17E+00	19,20	4.09E+01	22	6.17E+00	25	6.17E+00	25	4.89E-03		1.68E+00	28	4.89E-03	28

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		RCF in fresh wt (FW) (g COPC/g FW plant) / (g COPC/mL soil water)		Plant-soil bioconcentration factor for below ground produce (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for aboveground produce (HHRAP variable = Br _{ag}) (same value used for Br _{grain}) (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Plant-soil bioconcentration factor for forage and silage (g COPC/g DW plant) / (g COPC/g DW soil) (unitless)		Air-to-plant biotransfer factor in aboveground produce (HHRAP variable = Bv _{ag}) (g COPC/g DW plant)/ (g COPC/g air) (unitless)		LOG Bvol		Air-to-plant biotransfer factor in forage and silage (g COPC/g DW plant)/ (g COPC/g air) (unitless)	
CAS #	Compound name	RCF FW	Note	Br, root-veg	Note	Br, leafy-veg	Note	Br, forage	Note	Bv, leafy veg	Log Bvol	Note	Bv, forage	Note	
1634-04-4	methyl tert-butyl ether	1.07E+00	19,20	9.28E-01	22	7.84E+00	25	7.84E+00	25	1.80E-03	1.24E+00	28	1.80E-03	28	
75-56-9	Propylene oxide	8.52E-01	19,20	2.62E+01	22	8.38	25a	8.38	25a	4.89E-04	6.76E-01	28	4.89E-04	28	
33213-65-9	Endosulfan II	2.55E+01	18,20	4.56E+01	22	2.46E-01	25	2.46E-01	25	4.79E+01	5.67E+00	28	4.79E+01	28	
7446-09-5	Sulfur dioxide	8.21E-01	19,20	2.11E+02	22	7.24E+02	25	7.24E+02	25	3.13E-07	-2.52E+00	28	3.13E-07	28	
10102-44-0	Nitrogen dioxide	8.31E-01	19,20	1.15E+02	22	8.38E+01	25	8.38E+01	25	5.50E-07	-2.27E+00	28	5.50E-07	28	
Compounds evaluated for fugitive vap															
106-99-0	1,3-Butadiene	NA		NA		NA		NA		NA			NA		
110-82-7	Cyclohexane	NA		NA		NA		NA		NA			NA		

-- = Not applicable - compound did not have chronic human health toxicity data, or ecological risk assessment toxicity reference values (TRVs), and thus was not evaluated in the multiple pathway fate and transport modeling.

NA = Not applicable. Compound was only evaluated for the inhalation pathway in the human health risk assessment addressing potential fugitive emissions.

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biotransfer factor in milk (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)	LOG Ba,fat (Ba,fat in mg/kg fat / mg/day)		Biotransfer factor in beef (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in pork (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Bioconcentration factor in fish (L/kg FW OR unitless)	LOG BCF		Bioaccumulation factor in fish (mg COPC/kg FW tissue)/ (mg COPC/L total water column) OR (L water/kg FW tissue)	
CAS #	Compound name	Ba, milk	Log (Ba,fat)	Note	Ba, beef	Note	Ba, pork	Note	BCF, fish	log BCF	Note	BAF, fish	Note
563-58-6	1,1-Dichloropropene			--		--		--			--		--
95-63-6	1,2,4-Trimethylbenzene	4.70E-03	-9.30E-01	30a	2.23E-02	30b	2.70E-02	33	1.62E+02	2.21E+00	40b		
142-28-9	1,3-Dichloropropane	6.11E-04	-1.82E+00	30a	2.90E-03	30b	3.51E-03	33	6.92E+00	8.40E-01	40b		
108-60-1	2,2'-oxybis (1-Chloropropane)	1.22E-03	-1.52E+00	30a	5.80E-03	30b	7.02E-03	33	1.62E+01	1.21E+00	40b		
594-20-7	2,2-Dichloropropane	2.10E-03	-1.28E+00	30a	9.98E-03	30b	1.21E-02	33	3.54E+01	1.55E+00	40b		
625-86-5	2,5-Dimethylfuran	8.75E-04	-1.66E+00	30a	4.16E-03	30b	5.03E-03	33	1.06E+01	1.02E+00	40b		
2216-30-0	2,5-Dimethylheptane			--		--	0	--	0		--		--
17559-81-8	2,5-Dione, 3-hexene			--		--	0	--	0		--		--
78-93-3	2-Butanone	2.21E-05	-3.26E+00	30a	1.05E-04	30b	1.27E-04	33	3.16		40a	0	
95-49-8	2-Chlorotoluene	3.50E-03	-1.06E+00	30a	1.66E-02	30b	2.01E-02	33	8.58E+01	1.93E+00	40b	0	
591-78-6	2-Hexanone	2.14E-04	-2.27E+00	30a	1.02E-03	30b	1.23E-03	33	2.30E+00	3.63E-01	40b		
3221-61-2	2-Methyl octane			--	0	--		--			--		--
91-57-6	2-Methylnaphthalene	5.12E-03	-8.93E-01	30a	2.43E-02	30b	2.94E-02	33	2.01E+02	2.30E+00	40b		
34246-54-3	3-Ethyl benzaldehyde			--	0	--		--			--		--

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biotransfer factor in milk (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)	LOG Ba,fat (Ba,fat in mg/kg fat / mg/day)		Biotransfer factor in beef (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in pork (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Bioconcentration factor in fish (L/kg FW OR unitless)	LOG BCF		Bioaccumulation factor in fish (mg COPC/kg FW tissue)/ (mg COPC/L total water column) OR (L water/kg FW tissue)	
CAS #	Compound name	Ba, milk	Log (Ba,fat)	Note	Ba, beef	Note	Ba, pork	Note	BCF, fish	log BCF	Note	BAF, fish	Note
763-93-9	3-Hexen-2-one			--	0	--		--			--		--
625-33-2	3-Penten-2-one (ethylidene acetone)			--	0	--		--			--		--
141-79-7	3-Penten-2-one, 4- methyl			--		--		--			--		--
534-52-1	4,6-Dinitro-2- methylphenol	7.34E-04	-1.74E+00	30a	3.49E-03	30b	4.22E-03	33	8.56E+00	9.32E-01	40b		
106-43-4	4-Chlorotoluene	3.22E-03	-1.09E+00	30a	1.53E-02	30b	1.85E-02	33	7.31E+01	1.86E+00	40b		
4748-78-1	4-Ethyl benzaldehyde			--		--		--			--		--
301-02-0	9-Octadecenamide (oleamide)			--		--		--			--		--
208-96-8	Acenaphthylene	5.82E-03	-8.37E-01	30a	2.76E-02	30b	3.35E-02	33	2.86E+02	2.46E+00	40b		
7429-90-5	Aluminum	0.0002		31	0.0015	31	0	34	500		42		
92-87-5	Benzidine	3.76E-04	-2.03E+00	30a	1.79E-03	30b	2.16E-03	33	4.06E+00	6.09E-01	40b		
192-97-2	Benzo(e)pyrene			--		--		--			--		--
191-24-2	Benzo(g,h,i)perylene	6.19E-03	-8.10E-01	30a	2.94E-02	30b	3.56E-02	33	7.28E+04	4.86E+00	40b +.48		
93-58-3	Benzoic acid, methyl ester (methyl benzoate)	7.34E-04	-1.74E+00	30a	3.49E-03	30b	4.22E-03	33	8.56E+00	9.32E-01	40b		
111-91-1	Bis(2-chloroethoxy) methane	6.15E-05	-2.81E+00	30a	2.92E-04	30b	3.54E-04	33	3.16		40a		

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biotransfer factor in milk (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)	LOG Ba,fat (Ba,fat in mg/kg fat / mg/day)		Biotransfer factor in beef (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in pork (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Bioconcentration factor in fish (L/kg FW OR unitless)	LOG BCF		Bioaccumulation factor in fish (mg COPC/kg FW tissue)/ (mg COPC/L total water column) OR (L water/kg FW tissue)	
CAS #	Compound name	Ba, milk	Log (Ba,fat)	Note	Ba, beef	Note	Ba, pork	Note	BCF, fish	log BCF	Note	BAF, fish	Note
108-86-1	Bromobenzene	2.27E-03	-1.25E+00	30a	1.08E-02	30b	1.31E-02	33	4.00E+01	1.60E+00	40b		
74-97-5	Bromochloromethane			--	0	--		--			--		--
104-51-8	Butylbenzene, n-			--	0	--		--			--		--
135-98-8	Butylbenzene, sec			--		--		--			--		--
98-06-6	Butylbenzene, tert	5.85E-03	-8.35E-01	30a	2.78E-02	30b	3.37E-02	33	2.92E+02	2.46E+00	40b		
86-74-8	Carbazole	4.42E-03	-9.56E-01	30a	2.10E-02	30b	2.54E-02	33	1.41E+02	2.15E+00	40b		
7440-48-4	Cobalt	2.00E-03		31	0.02	31	0	34	300		42		
7440-50-8	Copper	1.50E-03		31	0.01	31	0	34	200		42		
2303-16-4	Diallate			--		--		--			--		--
132-64-9	Dibenzofuran	5.82E-03	-8.37E-01	30a	2.76E-02	30b	3.35E-02	33		2.46E+00		3.15E+02	41 (FCM =1.1)
122-39-4	Diphenylamine	3.75E-03	-1.03E+00	30a	1.78E-02	30b	2.16E-02	33	9.89E+01	2.00E+00	40b		
1031-07-8	Endosulfan sulfate	4.29E-03	-9.70E-01	30a	2.04E-02	30b	2.46E-02	33	1.31E+02	2.12E+00	40b		
7421-93-4	Endrin aldehyde	7.89E-03	-7.05E-01	30a	3.75E-02	30b	4.54E-02	33	9.91E+02	3.00E+00	40b		
53494-70-5	Endrin ketone			--		--		--			--		--

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biotransfer factor in milk (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)	LOG Ba,fat (Ba,fat in mg/kg fat / mg/day)		Biotransfer factor in beef (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in pork (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Bioconcentration factor in fish (L/kg FW OR unitless)	LOG BCF		Bioaccumulation factor in fish (mg COPC/kg FW tissue)/ (mg COPC/L total water column) OR (L water/kg FW tissue)	
CAS #	Compound name	Ba, milk	Log (Ba,fat)	Note	Ba, beef	Note	Ba, pork	Note	BCF, fish	log BCF	Note	BAF, fish	Note
76-13-1	Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane)	2.72E-03	-1.17E+00	30a	1.29E-02	30b	1.56E-02	33	5.41E+01	1.73E+00	40b		
74-88-4	Iodomethane	2.70E-04	-2.17E+00	30a	1.28E-03	30b	1.55E-03	33	2.90E+00	4.63E-01	40b		
99-87-6	Isopropyl toluene, p-	5.82E-03	-8.37E-01	30a	2.76E-02	30b	3.35E-02	33	2.86E+02	2.46E+00	40b		
7439-96-5	Manganese	3.50E-04		31	4.00E-04	31	0	34	400		42		
62-75-9	N-nitrosodimethylamine	2.51E-06	-4.20E+00	30a	1.19E-05	30b	1.44E-05	33	3.16		40a		
198-55-0	Perylene			--		--		--			--		--
2240-47-3	Phosphine imide, P,P,P-triphenyl			--		--		--			--	0	--
103-65-1	Propylbenzene, n-			--		--		--			--	0	--
7440-62-2	Vanadium	2.00E-05		31	2.50E-03	31	0	34	0		42a		
58-89-9	γ-BHC (Lindane)	4.08E-03	-9.91E-01	30a	1.94E-02	30b	2.35E-02	33	1.18E+02	2.07E+00	40b		
319-86-8	δ-BHC	5.96E-03	-8.27E-01	30a	2.83E-02	30b	3.43E-02	33	0.00E+00	2.49E+00		3.38E+02	41 (FCM=1.1)
110-54-3	1-Hexane (n-hexane)	5.12E-03	-8.93E-01	30a	2.43E-02	30b	2.94E-02	33	2.01E+02	2.30E+00	40b		
79-10-7	Acrylic Acid	1.63E-05	-3.39E+00	30a	7.73E-05	30b	9.36E-05	33	3.16		40c		
107-21-1	Ethylene Glycol	2.53E-07	-5.20E+00	30a	1.20E-06	30b	1.46E-06	33	3.16		40a		
80-62-6	Methyl methacrylate	2.14E-04	-2.27E+00	30a	1.02E-03	30b	1.23E-03	33	2.30E+00	3.63E-01	40b		

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biotransfer factor in milk (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)	LOG Ba,fat (Ba,fat in mg/kg fat / mg/day)		Biotransfer factor in beef (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in pork (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Bioconcentration factor in fish (L/kg FW OR unitless)	LOG BCF		Bioaccumulation factor in fish (mg COPC/kg FW tissue)/ (mg COPC/L total water column) OR (L water/kg FW tissue)	
CAS #	Compound name	Ba, milk	Log (Ba,fat)	Note	Ba, beef	Note	Ba, pork	Note	BCF, fish	log BCF	Note	BAF, fish	Note
1634-04-4	methyl tert-butyl ether	1.53E-04	-2.42E+00	30a	7.25E-04	30b	8.77E-04	33	1.67E+00	2.24E-01	40b		
75-56-9	Propylene oxide	1.19E-05	-3.53E+00	30a	5.63E-05	30b	6.82E-05	33	3.16		40a		
33213-65-9	Endosulfan II	4.77E-03	-9.24E-01	30a	2.27E-02	30b	2.74E-02	33	1.68E+02	2.23E+00	40b		
7446-09-5	Sulfur dioxide	1.62E-08	-6.39E+00	30a	7.68E-08	30b	9.30E-08	33	3.16		40a		
10102-44-0	Nitrogen dioxide	2.44E-06	-4.21E+00	30a	1.16E-05	30b	1.41E-05	33	3.16		40a		
Compounds evaluated for fugitive vap													
106-99-0	1,3-Butadiene	NA	NA		NA		NA		NA			NA	
110-82-7	Cyclohexane	NA	NA		NA		NA		NA			NA	

-- = Not applicable - compound did not have chronic human health toxicity data, or ecological risk assessment toxicity reference values (TRVs), and thus was not evaluated in the multiple pathway fate and transport modeling.

NA = Not applicable. Compound was only evaluated for the inhalation pathway in the human health risk assessment addressing potential fugitive emissions.

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biota-sediment accumulation factor in fish (mg COPC/kg lipid tissue)/(mg COPC/kg sediment) (unitless)		Plant-soil bioconcentration factor for grain (HHRAP variable = Br_{grain}) (same value used for Bra_g) (g COPC/g DW grain) / (g COPC/g DW soil) (unitless)		Biotransfer factor in eggs (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in chicken (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)	
CAS #	Compound name	BSAF, fish	Note	Br, grain	Note	Ba, egg	Note	Ba, chicken	Note
563-58-6	1,1-Dichloropropene		--		--		--		--
95-63-6	1,2,4-Trimethylbenzene			2.53E-01	37	9.40E-03	35b	1.65E-02	35a
142-28-9	1,3-Dichloropropane			2.70E+00	37	1.22E-03	35b	2.14E-03	35a
108-60-1	2,2'-oxybis (1-Chloropropane)			1.43E+00	37	2.44E-03	35b	4.27E-03	35a
594-20-7	2,2-Dichloropropane			7.95E-01	37	4.20E-03	35b	7.35E-03	35a
625-86-5	2,5-Dimethylfuran			1.96E+00	37	1.75E-03	35b	3.06E-03	35a
2216-30-0	2,5-Dimethylheptane		--		--		--		--
17559-81-8	2,5-Dione, 3-hexene		--		--		--		--
78-93-3	2-Butanone	0		8.38E+00	37	4.42E-05	35b	7.73E-05	35a
95-49-8	2-Chlorotoluene	0		4.09E-01	37	6.99E-03	35b	1.22E-02	35a
591-78-6	2-Hexanone			6.17E+00	37	4.28E-04	35b	7.49E-04	35a
3221-61-2	2-Methyl octane		--		--		--		--
91-57-6	2-Methylnaphthalene			2.16E-01	37	1.02E-02	35b	1.79E-02	35a
34246-54-3	3-Ethyl benzaldehyde		--		--		--		--

TABLE 1
CHEMICAL-SPECIFIC PARAMETERS FOR COMPOUNDS NOT IN USEPA'S HHRAP

		Biota-sediment accumulation factor in fish (mg COPC/kg lipid tissue)/(mg COPC/kg sediment) (unitless)		Plant-soil bioconcentration factor for grain (HHRAP variable = Br_{grain}) (same value used for Bra_g) (g COPC/g DW grain) / (g COPC/g DW soil) (unitless)		Biotransfer factor in eggs (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in chicken (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)	
CAS #	Compound name	BSAF, fish	Note	Br, grain	Note	Ba, egg	Note	Ba, chicken	Note
763-93-9	3-Hexen-2-one		--		--		--		--
625-33-2	3-Penten-2-one (ethylidene acetone)		--		--		--		--
141-79-7	3-Penten-2-one, 4-methyl		--		--		--		--
534-52-1	4,6-Dinitro-2-methylphenol			2.30E+00	37	1.47E-03	35b	2.57E-03	35a
106-43-4	4-Chlorotoluene			4.61E-01	37	6.43E-03	35b	1.13E-02	35a
4748-78-1	4-Ethyl benzaldehyde		--		--		--		--
301-02-0	9-Octadecenamide (oleamide)		--		--		--		--
208-96-8	Acenaphthylene			1.65E-01	37	1.16E-02	35b	2.04E-02	35a
7429-90-5	Aluminum			6.50E-04	38	0	36	0	36
92-87-5	Benzidine			4.03E+00	37	7.52E-04	35b	1.32E-03	35a
192-97-2	Benzo(e)pyrene		--		--		--		--
191-24-2	Benzo(g,h,i)perylene			5.93E-03	37	1.24E-02	35b	2.17E-02	35a
93-58-3	Benzoic acid, methyl ester (methyl benzoate)			2.30E+00	37	1.47E-03	35b	2.57E-03	35a
111-91-1	Bis(2-chloroethoxy) methane			8.38E+00	37	1.23E-04	35b	2.15E-04	35a

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CAS #	Compound name	BSAF, fish	Note	Br, grain	Note	Ba, egg	Note	Ba, chicken	Note
108-86-1	Bromobenzene			7.24E-01	37	4.54E-03	35b	7.95E-03	35a
74-97-5	Bromochloromethane		--		--		--		--
104-51-8	Butylbenzene, n-		--		--		--		--
135-98-8	Butylbenzene, sec		--		--		--		--
98-06-6	Butylbenzene, tert			1.63E-01	37	1.17E-02	35b	2.05E-02	35a
86-74-8	Carbazole			2.81E-01	37	8.85E-03	35b	1.55E-02	35a
7440-48-4	Cobalt			7.00E-03	38	0	36	0	36
7440-50-8	Copper			2.50E-01	38	0	36	0	36
2303-16-4	Diallate		--		--		--		--
132-64-9	Dibenzofuran			1.65E-01	37	1.16E-02	35b	2.04E-02	35a
122-39-4	Diphenylamine			3.67E-01	37	7.50E-03	35b	1.31E-02	35a
1031-07-8	Endosulfan sulfate			2.97E-01	37	8.57E-03	35b	1.50E-02	35a
7421-93-4	Endrin aldehyde			6.51E-02	37	1.58E-02	35b	2.76E-02	35a
53494-70-5	Endrin ketone		--		--		--		--

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CAS #	Compound name	BSAF, fish	Note	Br, grain	Note	Ba, egg	Note	Ba, chicken	Note
76-13-1	Freon 113 (1,1,2-trichloro-1,2,2-trifluoroethane)			5.77E-01	37	5.44E-03	35b	9.52E-03	35a
74-88-4	Iodomethane			5.19E+00	37	5.41E-04	35b	9.46E-04	35a
99-87-6	Isopropyl toluene, p-			1.65E-01	37	1.16E-02	35b	2.04E-02	35a
7439-96-5	Manganese			5.00E-02	38	0	36	0	36
62-75-9	N-nitrosodimethylamine			8.38E+00	37	5.02E-06	35b	8.79E-06	35a
198-55-0	Perylene		--		--		--		--
2240-47-3	Phosphine imide, P,P,P-triphenyl		--		--		--		--
103-65-1	Propylbenzene, n-		--		--		--		--
7440-62-2	Vanadium			3.00E-03	38	0	36	0	36
58-89-9	γ-BHC (Lindane)			3.22E-01	37	8.17E-03	35b	1.43E-02	35a
319-86-8	δ-BHC			1.57E-01	37	1.19E-02	35b	2.09E-02	35a
110-54-3	1-Hexane (n-hexane)			2.16E-01	37	1.02E-02	35b	1.79E-02	35a
79-10-7	Acrylic Acid			8.38E+00	37	3.26E-05	35b	5.70E-05	35a
107-21-1	Ethylene Glycol			8.38E+00	37	5.07E-07	35b	8.87E-07	35a
80-62-6	Methyl methacrylate			6.17E+00	37	4.28E-04	35b	7.49E-04	35a

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		Biota-sediment accumulation factor in fish (mg COPC/kg lipid tissue)/(mg COPC/kg sediment) (unitless)		Plant-soil bioconcentration factor for grain (HHRAP variable = Br_{grain}) (same value used for Br_g) (g COPC/g DW grain) / (g COPC/g DW soil) (unitless)		Biotransfer factor in eggs (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)		Biotransfer factor in chicken (mg COPC/kg FW tissue)/ (mg COPC/day) OR (day/kg FW tissue)	
CAS #	Compound name	BSAF, fish	Note	Br, grain	Note	Ba, egg	Note	Ba, chicken	Note
1634-04-4	methyl tert-butyl ether			7.84E+00	37	3.05E-04	35b	5.34E-04	35a
75-56-9	Propylene oxide			8.38E+00	37	2.37E-05	35b	4.15E-05	35a
33213-65-9	Endosulfan II			2.46E-01	37	9.54E-03	35b	1.67E-02	35a
7446-09-5	Sulfur dioxide			7.24E+02	37	3.24E-08	35b	5.66E-08	35a
10102-44-0	Nitrogen dioxide			8.38E+01	37	4.89E-06	35b	8.56E-06	35a
<i>Compounds evaluated for fugitive vap</i>									
106-99-0	1,3-Butadiene	NA		NA		NA		NA	
110-82-7	Cyclohexane	NA		NA		NA		NA	

-- = Not applicable - compound did not have chronic human health toxicity data, or ecological risk assessment toxicity reference values (TRVs), and thus was not evaluated in the multiple pathway fate and transport modeling.

NA = Not applicable. Compound was only evaluated for the inhalation pathway in the human health risk assessment addressing potential fugitive emissions.

TABLE 2

**REFERENCES FOR NOTES INCLUDED IN
CHEMICAL-PHYSICAL PROPERTIES TABLE**

TABLE 2
REFERENCES FOR NOTES INCLUDED IN CHEMICAL-PHYSICAL PROPERTIES TABLE

Note	Parameter	Description
1	Molecular weight (MW), melting point (Tm), vapor pressure (VP), water solubility (S), Henry's law constant (H), log octanol:water partition coefficient (log Kow), soil:water partition coefficient (Kd)	Superfund Chemical Data Matrix – USEPA (2005) Appendix A-2 recommended source
2	Molecular weight (MW), melting point (Tm), vapor pressure (VP), water solubility (S), Henry's law constant (H), log octanol:water partition coefficient (log Kow)	CHEMFATE (www.esc.syrres.com/eSc/chemfate.htm) – USEPA (2005) Appendix A-2 recommended source
3	Molecular weight (MW), melting point (Tm), vapor pressure (VP), water solubility (S), Henry's law constant (H), log octanol:water partition coefficient (log Kow)	Physprop (www.syrres.com/eSc/physdemo.htm) - USEPA (2005) Appendix A-2 recommended source
3a	Henry's law constant (H)	As directed in HHRAP, for metals, if no value is provided in sources 1, 2 or 3, assign a value of 0 (page A-2-8)
5	Organic carbon:water partition coefficient (Koc), soil:water partition coefficient (Kd)	USEPA's Soil Screening Guidance - USEPA (2005) Appendix A-2 recommended source
6	Air diffusivity (Da), water diffusivity (Dw)	USEPA's Water9 Model - USEPA (2005) Appendix A-2 recommended source
6a	Air diffusivity (Da), water diffusivity (Dw)	Per HHRAP, if no value is available in USEPA's WATER9 model, calculate based on molecular weight - HHRAP Equations A-2-4 and A-2-5
7	Soil:water partition coefficient (Kd)	Baes et al. (1984) - USEPA (2005) Appendix A-2 recommended source
8	Water solubility (S)	For compounds that are miscible, use USEPA default of 1E+6 mg/L
9	Organic carbon:water partition coefficient (Koc)	Calculate according to HHRAP Equation A-2-7

TABLE 2
REFERENCES FOR NOTES INCLUDED IN CHEMICAL-PHYSICAL PROPERTIES TABLE

Note	Parameter	Description
10	Organic carbon:water partition coefficient (K_{oc})	Calculate according to HHRAP Equation A-2-8
11	Organic carbon:water partition coefficient (K_{oc})	According to HHRAP, default value for K_{oc} for metals is 0.
12	Organic carbon:water partition coefficient (K_{oc})	IWEM default chemical properties data. www.epa.gov/epaoswer/non-hw/industd/iwem_tbd.htm .
13	Soil:water partition coefficient (K_{ds})	Calculate according to HHRAP Equation A-2-10
14	Suspended sediment:water partition coefficient ($K_{d_{sw}}$)	Calculate according to HHRAP Equation A-2-11
14b	Suspended sediment:water partition coefficient ($K_{d_{sw}}$), benthic sediment:water partition coefficient ($K_{d_{bs}}$)	According to HHRAP, for metals, assume $K_{d_{sw}}$ and $K_{d_{bs}} = K_{ds}$
15	Benthic sediment:water partition coefficient ($K_{d_{bs}}$)	Calculate according to HHRAP Equation A-2-12
16	Fraction vapor (f_v)	Calculate according to HHRAP Equation A-2-1
16a	Fraction vapor (f_v)	According to HHRAP, for metals, assume $f_v = 0$
17	Fraction vapor (f_v)	Calculate according to HHRAP Equations A-2-2 and A-2-1
18	Log root concentration factor (RCF)	Calculate according to HHRAP Equation A-2-14
19	Log root concentration factor (RCF)	Calculate according to HHRAP Equation A-2-15
20	Root concentration factor (RCF_{FW})	Calculate according to HHRAP Equation A-2-16
21	Root concentration factor (RCF_{FW})	According to HHRAP, set $RCF = 6.39$ if $\log K_{ow} < -0.57$
21a	Root concentration factor (RCF_{FW})	According to HHRAP, for metals, assume $RCF = 0$
22	Soil-to-plant bioconcentration factor for below ground produce ($Br_{rootveg}$)	Calculate according to HHRAP Equation A-2-16

TABLE 2
REFERENCES FOR NOTES INCLUDED IN CHEMICAL-PHYSICAL PROPERTIES TABLE

Note	Parameter	Description
23	Soil-to-plant bioconcentration factor for below ground produce ($Br_{rootveg}$)	According to HHRAP, values for metals obtained from Baes et al. 1984
24	Melting point (T_m), vapor pressure (VP), water solubility (S), Henry's law constant (H), log octanol:water partition coefficient (log Kow), organic carbon:water partition coefficient (Koc)	USEPA's EpiSuite™.v3 Program (Estimation Programs Interface) (http://www.epa.gov/oppt/exposure/pubs/episuite.htm)
25	Soil-to-plant bioconcentration factor for aboveground produce (Br_{ag}), soil-to-plant bioconcentration factor for forage and silage (Br_{forage})	Calculate according to HHRAP Equations A-2-17 and A-2-18 (equations are identical for the produce types)
25a	Soil-to-plant bioconcentration factor for aboveground produce (Br_{ag}), soil-to-plant bioconcentration factor for forage and silage (Br_{forage})	According to HHRAP, set Br_{ag} and $Br_{forage} = 8.38$ if $\log Kow < 1.15$
26	Soil-to-plant bioconcentration factor for forage and silage (Br_{forage})	For metals, use values in Baes et al. 1984 for B_v (vegetative growth-leaves and stems, Figure 2.1 in Baes)
27	Soil-to-plant bioconcentration factor for aboveground produce (Br_{ag})	For metals, use weighted average of values in Baes et al. 1984 for B_v (vegetative growth-leaves and stems) and Br (reproductive growth – fruit, seeds, tubers, Figure 2.2 in Baes), weighting by consumption (pp. A-2-18 to A-2-19)
28	Air-to-plant biotransfer factor in aboveground produce (Bv_{ag}), air-to-plant biotransfer factor for forage and silage (Bv_{forage})	Calculate according to HHRAP Equations A-2-19 and A-2-20
29	Air-to-plant biotransfer factor in aboveground produce (Bv_{ag}), air-to-plant biotransfer factor for forage and silage (Bv_{forage})	According to HHRAP, for metals, assume air-to-leaf transfer = 0

TABLE 2
REFERENCES FOR NOTES INCLUDED IN CHEMICAL-PHYSICAL PROPERTIES TABLE

Note	Parameter	Description
30	Log fat biotransfer coefficient (Ba_{fat})	Calculate according to HHRAP Equation A-2-21
30a	Biotransfer factor in milk (Ba_{milk})	Calculate according to HHRAP Equation A-2-22 (not used because dairy milk pathway was not evaluated – see main text)
30b	Biotransfer factor in beef (Ba_{beef})	Calculate according to HHRAP Equation A-2-23
31	Biotransfer factor in milk (Ba_{milk}), biotransfer factor in beef (Ba_{beef})	According to HHRAP, values for metals obtained from Baes et al. 1984 (Figure 2.25 for beef and Figure 2.24 for milk)
33	Biotransfer factor in pork (Ba_{pork})	Calculate according to HHRAP Equation A-2-26
34	Biotransfer factor in pork (Ba_{pork})	According to HHRAP, values for metals assumed to be 0
35a	Biotransfer factor in chicken/poultry ($Ba_{chicken}$)	Calculate according to HHRAP Equation A-2-27
35b	Biotransfer factor in eggs (Ba_{egg})	Calculate according to HHRAP Equation A-2-28
36	Biotransfer factor in eggs (Ba_{egg}), biotransfer factor in chicken/poultry ($Ba_{chicken}$)	Following HHRAP guidance, for metals, $Ba_{chicken}$ and Ba_{egg} assumed to be 0
37	Soil-to-plant bioconcentration factor for grain (Br_{grain})	Use Br_{forage} values (p. A-2-17)
38	Soil-to-plant bioconcentration factor for grain (Br_{grain})	For metals, use values in Baes et al. for Br (reproductive growth – fruit, seeds, tubers, Figure 2.2 in Baes)
40a	Fish bioconcentration factor (BCF)	Calculate according to HHRAP Equation A-2-27
40b	Fish bioconcentration factor (BCF)	Calculate according to HHRAP Equation A-2-28
40c	Fish bioconcentration factor (BCF)	Calculate according to HHRAP Equation A-2-31
41	Fish bioconcentration factor (BCF)	Calculate according to HHRAP Equation A-2-28 multiplied by a Food Chain Multiplier (FCM) obtained from USEPA's 1999 Screening Level Ecological Risk Assessment Protocol (Table 5-2)
42	Fish bioconcentration factor (BCF)	Values for metals obtained from Oak Ridge National Laboratory, Risk Assessment Information System (RAIS). Rais.ornl.gov/homepage/rap_tool.shtml

TABLE 2
REFERENCES FOR NOTES INCLUDED IN CHEMICAL-PHYSICAL PROPERTIES TABLE

Note	Parameter	Description
42a	Fish bioconcentration factor (BCF)	A bioconcentration factor for vanadium was not provided in RAIS. Fish uptake is low for this compound (Miramand, Fowler and Guary. 2004. Experimental study on vanadium transfer in the benthic fish <i>Gobius minutus</i> . Marine Biol. 114:349-353)
43	Vapor pressure (VP), organic carbon:water partition coefficient (Koc)	Following HHRAP guidance for metals, a default value of 0 is used
44	Soil loss constant due to biotic and abiotic degradation (Ksg)	Assume a conservative default value of 0
45	Soil loss constant due to biotic and abiotic degradation (Ksg)	Calculate according to HHRAP Equation A-2-13, based on data in ATSDR. 2001. Toxicological Profile for Benzidine