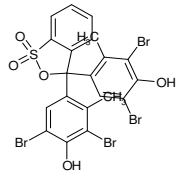
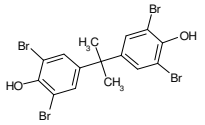
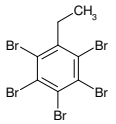
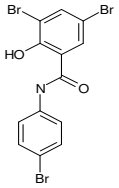
Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000076-60-8	76608	
	000079-94-7	79947	
	000085-22-3	85223	
	000087-10-5	87105	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000076-60-8	O=S(=O)(OC(c1cccc2)(c(c(c(c(O)c3Br)Br)C)c3)c(c(c(c(O)c4Br)Br)C)c4)c12	Br	2.87E-17	3.83E-15
000079-94-7	Oc(c(cc(c1)C(c(cc(c(O)c2Br)Br)c2)(C)C)Br)c1Br	Br	3.46E-11	4.61E-09
000085-22-3	c(c(c(c(c1Br)Br)Br)Br)(c1Br)CC	Br	4.65E-06	6.20E-04
000087-10-5	O=C(Nc(ccc(c1)Br)c1)c(c(O)c(cc2Br)Br)c2	Br	1.72E-11	2.29E-09

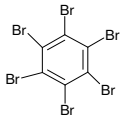
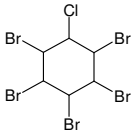
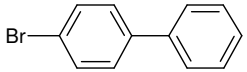
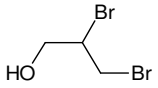
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000076-60-8	2.46	-16.58	7.86	24.44	1699	3.230193379
000079-94-7	3.62	-11.02	7.20	18.22	13550	4.131939295
000085-22-3	9.30	-3.49	7.48	10.97	14140	4.150449409
000087-10-5	2.73	-9.38	5.97	15.35	3121	3.494293769

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000076-60-8	Bromocresol Green. Pigment and dye. May be analysablel by GC-MS after derivatization or directly by LC-MS ESI	phenol	N	N	Y
000079-94-7	Methodology exists for TBBPA	phenol	Y	N	Y
000085-22-3	PBEB. Flame retardant use. Measured in Great Lakes air. Current production if any is below TSCA limit.	neutral	Y	Y	
000087-10-5	tribromsalan. Antimicrobial and pesticide	phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000076-60-8	Y?			N					
000079-94-7	Y			N	50	100	500	500	500
000085-22-3				N	0.5				
000087-10-5	Y?			N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000076-60-8		Y	0.042	Fish 96-hour LC_{50} (mg/L)	
000079-94-7	500	Y	2.37E-01	Fish, 96-hour LC_{50} (mg/L)	Low-moderate
000085-22-3	–	Y	1.51E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000087-10-5	–	Y	2.37E-01	Fish, 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000076-60-8	76608		Phenols
000079-94-7	79947		Neutral Organics
000085-22-3	85223		Esters
000087-10-5	87105		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000087-82-1	87821	
Top 10 brominated	000087-84-3	87843	
	000092-66-0	92660	
	000096-13-9	96139	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000087-82-1	c(c(c(c(c1Br)Br)Br)Br)(c1Br)Br	Br	1.68E-08	2.24E-06
000087-84-3	BrC(C(C(Br)C(Br)C1Br)Cl)C1Br	Br	3.46E-06	4.61E-04
000092-66-0	c(ccc(c(cccc1)c1)c2)(c2)Br	Br	2.61E-04	3.48E-02
000096-13-9	OCC(Br)CBr	Br	2.48E-02	3.31E+00

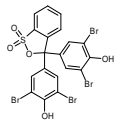
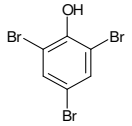
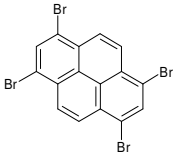
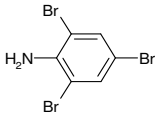
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000087-82-1	934.15	-4.06	7.33	11.39	9417	3.97391257
000087-84-3	15.71	-4.41	4.71	9.12	860	2.934397441
000092-66-0	3.09	-2.17	4.65	6.82	1316	3.119255889
000096-13-9	5.16	-6.59	0.96	7.55	3	0.499961866

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000087-82-1	Analysable with chlorobenzenes. Limited measurements in the Great Lakes	neutral	Y	Y	
000087-84-3	Analysable with HCHs	neutral	N	Y	
000092-66-0	related to now banned PBBs	neutral	N	Y	
000096-13-9	very volatile but probably amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000087-82-1				N				0.5	
000087-84-3				N			0.5		0.5
000092-66-0				N					
000096-13-9				N	10		0.5		0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000087-82-1	–	Y	9.64E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
000087-84-3	–	Y	4.40E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
000092-66-0		Y	1.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
000096-13-9	–	Y	114.271	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000087-82-1	87821		Neutral Organics
000087-84-3	87843		Esters
000092-66-0	92660		Neutral Organics
000096-13-9	96139		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000115-39-9	115399	
	000118-79-6	118796	
Top 10 brominated	000128-63-2	128632	
	000147-82-0	147820	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000115-39-9	O=S(=O)(OC(c1cccc2)(c(cc(c(O)c3Br)Br)c3)c(cc(c(O)c4Br)Br)c4)c12	Br	2.70E-17	3.60E-15
000118-79-6	Oc(c(cc(c1)Br)Br)c1Br	Br	3.03E-04	4.04E-02
000128-63-2	c(c(c(c(cc1Br)Br)cc2)c1cc3)(c2c(cc4Br)Br)c34	Br	4.06E-10	5.41E-08
000147-82-0	Nc(c(cc(c1)Br)Br)c1Br	Br	0.000212	0.028264342

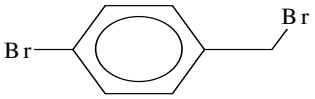
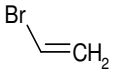
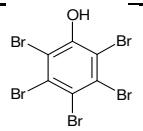
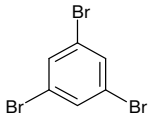
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000115-39-9	3.02	-16.67	6.77	23.44	12890	4.110252917
000118-79-6	22.52	-5.84	4.18	10.02	120	2.080265627
000128-63-2	6.57	-5.07	8.49	13.56	2424	3.384532615
000147-82-0	161.0769228	-5.30938953	3.75	5.665102142	152.9	2.184

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000115-39-9	looks very persistent but not in CUS and 0 to <1T in DSL. Several similar structures - use?	phenol	N	N	Y
000118-79-6	Flame retardant and intermediate. Also degradation product of several current use BFRs	phenol	Y	N	Y
000128-63-2	Tetrabromopyrene. Possible intermediate rather than BFR. Could be very light sensitive	neutral	N	Y	
000147-82-0	P - tribromo	amine	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000115-39-9	Y?			N					
000118-79-6	Y?			N	50	50	50	50	50
000128-63-2				N	0.5	1	10		1
000147-82-0				N	0.5	1			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000115-39-9		Y	0.02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000118-79-6	50	Y	2.37E+00	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000128-63-2	0.5	N	8.54E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
000147-82-0		Y	5.047	Fish 96-hour LC_{50} (mg/L)	moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000115-39-9	115399		Neutral Organics
000118-79-6	118796		Vinyl/Allyl Halides
000128-63-2	128632		Phenols (dinitro)
000147-82-0	147820	airbreather	Halo ethers

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000589-15-1	589151	
	000593-60-2	593602	
	000608-71-9	608719	
	000626-39-1	626391	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000589-15-1	BrCc(ccc(c1)Br)c1	Br	1.47E-02	1.96E+00
000593-60-2	BrC=C	Br	1.05E+03	1.40E+05
000608-71-9	Oc(c(c(c(c1Br)Br)Br)Br)c1Br	Br	5.08E-08	6.77E-06
000626-39-1	c(cc(cc1Br)Br)(c1)Br	Br	9.56E-04	1.27E-01

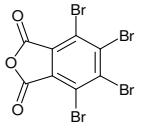
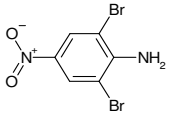
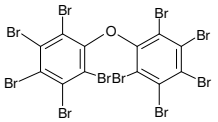
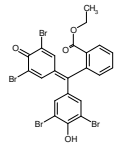
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000589-15-1	10.11	-2.95	3.77	6.72	161	2.205745541
000593-60-2	1.51	-0.30	1.52	1.82	3	0.508933526
000608-71-9	23.72	-6.64	5.96	12.60	3100	3.491361694
000626-39-1	21.99	-1.86	4.66	6.52	593	2.772688355

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000589-15-1	Analysable with other bromo/chlorobenzenes	neutral	N	Y	
000593-60-2	Vinyl bromide. Occupational measurements	neutral	N	Y	
000608-71-9	pentabromophenol. Flame retardant and intermediate.	phenol	N	N	Y
000626-39-1	Analysable with other bromo/chlorobenzenes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000589-15-1				N					0.5
000593-60-2				N	10		0.5		
000608-71-9	Y			N					
000626-39-1				N	0.5	1			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000589-15-1	0.5	Y	0.265	Fish 96-hour LC_{50} (mg/L)	
000593-60-2	–	Y	4.27E+00	Fish 96-hour LC_{50} (mg/L)	Moderate
000608-71-9	–	Y	0.261	Fish 96-hour LC_{50} (mg/L)	Moderate
000626-39-1	–	Y	4.90E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000589-15-1	589151		Neutral Organics
000593-60-2	593602		Vinyl/Allyl Halides
000608-71-9	608719		Neutral Organics
000626-39-1	626391		Esters + Phenols + Salicylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000632-79-1	632791	
	000827-94-1	827941	
	001163-19-5	1163195	
	001176-74-5	1176745	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000632-79-1	O=C(OC(=O)c1c(c(c(c2Br)Br)Br)Br)c12	Br	2.03E-08	2.71E-06
000827-94-1	O=N(=O)c(cc(c(N)c1Br)Br)c1	Br	0.0000146	0.001946507
001163-19-5	O(c(c(c(c(c1Br)Br)Br)Br)c1Br)c(c(c(c(c2Br)Br)Br)Br)c2Br	Br	4.67E-12	6.23E-10
001176-74-5	C1=C(Br)C(=O)C(Br)=CC1=C(c2ccccc2C(=O)OCC)c3cc(Br)c(O)c(Br)c3	Br	2.22E-15	2.96E-13

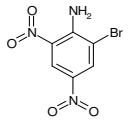
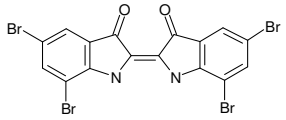
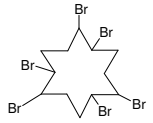
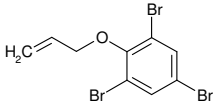
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000632-79-1	438.54	-5.18	5.63	10.81	4307	3.634174872
000827-94-1	1160.479062	-7.313023815	3.25	7.168736426	63.62	1.804
001163-19-5	317.58	-6.31	12.11	18.42	3	0.499961866
001176-74-5	0.06	-14.40	6.40	20.80	6719	3.827304641

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000632-79-1	hydrolysis to acid - flame retardant that is covalently bonded in polymer? Large production - monomer in polymer?	acid	N	N	
000827-94-1	P - two Br, one Nitro	neutral	N	Y?	
001163-19-5	low predicted BCF. - already an emerging contaminant - does it lose its bromines to become more B?	neutral	Y	Y	
001176-74-5	Pigment and dye. Tetrabromophenolphthalein Ethyl Ester. May be amenable to GC analysis after derivatization	phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000632-79-1		tetrabromophthalic acid	Y	N	10	10	50	50	50
000827-94-1				N	0.5	0.5	0.5	0.5	
001163-19-5				Y	50	50	100	100	100
001176-74-5		Phenyl Carboxylate	Y	N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000632-79-1	50	Y	3.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000827-94-1		Y	1.06E+01	Fish 96-hour LC_{50} (mg/L)	High-moderate
001163-19-5	100	N	4.72E-11	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
001176-74-5	–	Y	2.72E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000632-79-1	632791		Esters
000827-94-1	827941	airbreather	Neutral Organics
001163-19-5	1163195		Neutral Organics
001176-74-5	1176745		haloketones

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001817-73-8	1817738	
	002475-31-2	2475312	
Top 10 brominated	003194-55-6	3194556	
	003278-89-5	3278895	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001817-73-8	O=N(=O)c(cc(N(=O)=O)c(N)c1Br)c1	Br	0.00000202	0.000269311
002475-31-2	O=C(c(c(N1)c(cc2Br)Br)c2)C1=C(Nc(c3cc(c4)Br)c4Br)C3=O	Br	1.16E-12	1.55E-10
003194-55-6	BrC(C(Br)CCC(Br)C(Br)CCC(Br)C(Br)C1)C1	Br	1.68E-08	2.24E-06
003278-89-5	O(c(c(cc(c1)Br)Br)c1Br)CC=C	Br	1.01E-04	1.35E-02

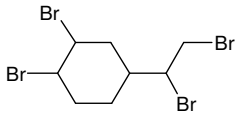
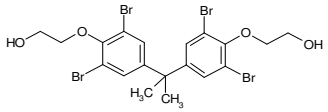
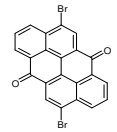
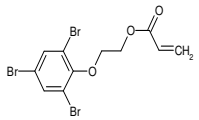
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
001817-73-8	8362.253355	-7.97695107	2.73	7.312663682	25.07	1.399
002475-31-2	1.42	-14.29	6.67	20.96	3972	3.59900924
003194-55-6	2.13	-4.15	7.74	11.89	6211	3.793161529
003278-89-5	0.25	-3.97	5.59	9.56	4019	3.604118006

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001817-73-8	P - one Br, two Nitro	neutral	N	Y?	
002475-31-2	May be analysable by GC-MS	neutral	N	Y	
003194-55-6	Hexabromocyclododecane. Limited Great Lakes measurements. Possible penta BDE replacement	neutral	Y	Y	
003278-89-5	Analysable with other bromo/chlorobenzenes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001817-73-8				N	10	10	1	0.5	
002475-31-2				N			0.5	0.5	
003194-55-6				Y	10	10	50	50	50
003278-89-5		Tribromophenol	Y	N		0.5	0.5	1	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001817-73-8	–	Y	5.81	Fish 96-hour LC_{50} (mg/L)	moderate
002475-31-2		Y	9.85E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003194-55-6	50	Y	9.17E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003278-89-5	0.5	Y	0.016	Fish 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
001817-73-8	1817738	airbreather	Neutral Organics
002475-31-2	2475312		Neutral Organics
003194-55-6	3194556		Neutral Organics
003278-89-5	3278895		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 brominated	003322-93-8	3322938	
	004162-45-2	4162452	
	004378-61-4	4378614	
	007347-19-5	7347195	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
003322-93-8	BrCC(Br)C(CCC(Br)C1Br)C1	Br	1.05E-04	1.40E-02
004162-45-2	O(c(c(cc(c1)C(c(cc(c(OCCO)c2Br)Br)c2)(C)C)Br)c1Br)CCO	Br	3.93E-14	5.24E-12
004378-61-4	O=C(c(c(c(c(c1Br)ccc2)c2C(=O)c3cc(c(c45)ccc6)Br)c34)c1)c56	Br	7.03E-13	9.37E-11
007347-19-5	O=C(OCCOc(c(cc(c1)Br)Br)c1Br)C=C	Br	2.43E-06	3.24E-04

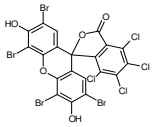
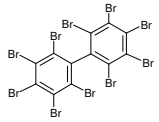
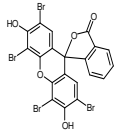
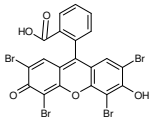
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
003322-93-8	2.20	-2.77	5.24	8.01	2153	3.33304403
004162-45-2	0.42	-11.14	6.78	17.92	7479	3.873843533
004378-61-4	1.51	-10.16	7.13	17.29	6110	3.78604121
007347-19-5	0.53	-6.86	5.13	11.99	1780	3.250420002

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
003322-93-8	Limited environmental measurements. Production volume in the 10,000-500,000 pounds/year range for all 5 reporting years of IUR/CUS and appears to be both persistent (P) and bioaccumulative (B) based upon QSARs.	neutral	N	Y	
004162-45-2	In Fireguard 3600; should degrade to TBBPA	neutral	N	N	
004378-61-4	Pigment Red 168; may be amenable to GC-MS or LC-MS	neutral	N	Y	
007347-19-5	Analysable with other bromo/chlorobenzenes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
003322-93-8				N	0.5	0.5	0.5	0.5	0.5
004162-45-2		TBBPA	Y	N	0.5	0.5	0.5	0.5	
004378-61-4				N	0.5	0.01	0.5	0.5	
007347-19-5		Tribromophenol	Y	N					0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
003322-93-8	–	Y	8.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
004162-45-2	–	Y	1.43E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
004378-61-4		Y	3.84E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
007347-19-5	1	Y	1.065	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
003322-93-8	3322938		Neutral Organics
004162-45-2	4162452		Neutral Organics
004378-61-4	4378614		Acrylates
007347-19-5	7347195		Esters

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	013473-26-2	13473262	
	013654-09-6	13654096	
	015086-94-9	15086949	
	017372-87-1	17372871	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
013473-26-2	O=C(OC(c(c(Oc1c(c(O)c(c2)Br)Br)c(c(O)c3Br)Br)c3)(c12)c4c(c(c(c5Cl)Cl)Cl)Cl)c45	Br	3.37E-20	4.49296E-18
013654-09-6	c(c(c(c(c1Br)Br)Br)Br)(c1c(c(c(c(c2Br)Br)Br)Br)c2Br)Br	Br	1.11E-14	1.48E-12
015086-94-9	O=C(OC(c(c(Oc1c(c(O)c(c2)Br)Br)c(c(O)c3Br)Br)c3)(c12)c4cccc5)c45	Br	1.94E-17	2.59E-15
017372-87-1	c12OC4=C(Br)C(=O)C(Br)=CC4=C(c3c(C(=O)O[Na])cccc3)c1cc(Br)c(O[Na])c2Br	Br	2.54E-20	3.38639E-18

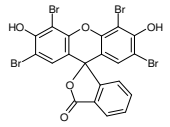
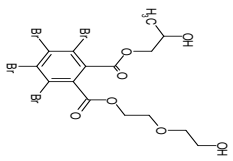
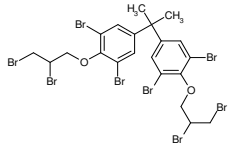
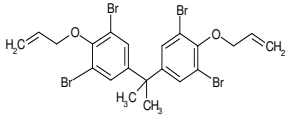
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
013473-26-2	65.26035334	-16.55798211	9.49	22.65369472	10.01	1.000
013654-09-6	852.27	-5.77	12.66	18.43	3	0.499961866
015086-94-9	1.87	-16.04	6.91	22.95	16640	4.221153322
017372-87-1	4.017799842	-17.57968491	-1.68	12.50539752	3.162	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
013473-26-2	Several Halogens, but has an ester - P? Maybe B. Use - spiro intermediate?	neutral	N	N	
013654-09-6	1,1 -Biphenyl, 2,2 ,3,3 ,4,4 ,5,5 ,6,6 -decabromo-	neutral	N	Y	
015086-94-9	May yield bromophenol degradation products	phenol	N	N	
017372-87-1	Dye May be P but not B - check spiro compds	Phenol	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
013473-26-2	Y			N		0.5	0.5	0.5	0.5
013654-09-6				N		0.5			
015086-94-9	Y			N	0.5	0.5	0.5	0.5	
017372-87-1	Y			N	0.5	0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
013473-26-2		Y	0.003	Fish 96-hour LC_{50} (mg/L)	
013654-09-6	–	N	9.54E-12	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
015086-94-9		Y	0.015	Mysid Shrimp 96-hour LC_{50} (mg/L)	
017372-87-1		Y	1.00E+05	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
013473-26-2	13473262	MPV	Acrylates
013654-09-6	13654096		Neutral Organics
015086-94-9	15086949		Acid Chloride/Halide
017372-87-1	17372871	MPV	Acid Chloride/Halide

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	018472-87-2	18472872	
	020566-35-2	20566352	
	021850-44-2	21850442	
	025327-89-3	25327893	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
018472-87-2	[Na]Oc1c(Br)c2Oc3c(Br)c(O[Na])c(Br)cc3C(OC(=O)c4c(Cl)c5Cl)(c4c(Cl)c5Cl)c2cc1Br	Br	2.34E-23	3.11974E-21
020566-35-2	O=C(OCCOCCO)c(c(c(c(c1Br)Br)Br)C(=O)OCC(O)C)c1Br	Br	2.37E-14	3.16E-12
021850-44-2	O(c(c(cc(c1)C(c(cc(c(OCC(Br)CBr)c2Br)Br)c2)(C)C)Br)c1Br)CC(Br)CBr	Br	6.36E-15	8.48E-13
025327-89-3	O(c(c(cc(c1)C(c(cc(c(OCC=C)c2Br)Br)c2)(C)C)Br)c1Br)CC=C	Br	1.99E-09	2.65E-07

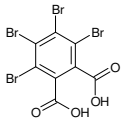
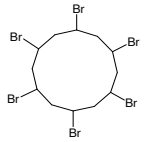
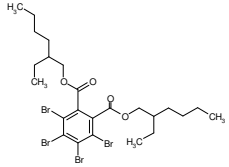
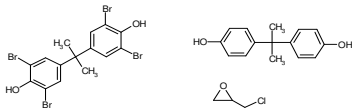
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
018472-87-2	61.79470973	-16.05613232	5.47	18.13184493	10.01	1.000
020566-35-2	0.35	-13.95	3.83	17.78	39	1.59571662
021850-44-2	1.02	-9.78	11.52	21.30	3	0.499961866
025327-89-3	0.12	-5.28	10.02	15.30	5	0.676967814

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
018472-87-2	Several Br - P. Dye intermediate - spiro compounds	Phenol	N	N	
020566-35-2	Replacement product for penta BDE. Great Lakes PHT4-DIOL/70;2-(2-Hydroxyethoxy) ethyl-2-hydroxypropyl-3,4,5,6-tetrabromo phthalate; may be amendable to GC-MS	neutral	N	Y	
021850-44-2	Derivative of tetrabromobisphenol A - ether with 4 more Br's; may be amenable to GC-MS analysis	neutral	N	Y	
025327-89-3	Derivative of tetrabromobisphenol A - ether with 4 more Br's; may be amenable to GC-MS analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
018472-87-2	Y			N		0.5	0.5	0.5	0.5
020566-35-2	Y?	tetrabromophthalic acid	Y	N	0.5	0.5		0.5	0.5
021850-44-2	Y?	TBBPA	Y	N			0.5	0.5	
025327-89-3		TBBPA	Y	N	500	500	500	5000	5000

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
018472-87-2		Y	1.748	Fish 96-hour LC_{50} (mg/L)	
020566-35-2	–	Y	9.97E+00	Fish 96-hour LC_{50} (mg/L)	
021850-44-2	10	N	4.10E-02	Fish 96-hour LC_{50} (mg/L)	
025327-89-3	0.5	N	8.67E-05	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
018472-87-2	18472872	MPV	Neutral Organics
020566-35-2	20566352		Neutral Organics
021850-44-2	21850442		Esters
025327-89-3	25327893		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	025357-79-3	25357793	
	025637-99-4	25637994	
Top 10 brominated	026040-51-7	26040517	
	026265-08-7	26265087	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
025357-79-3	[Na]OC(=O)c1c(Br)c(Br)c(Br)c(Br)c1C(=O)O[Na]	Br	9.89E-14	1.32E-11
025637-99-4	BrC1CC(CC(CC(CC(CC(C1)Br)Br)Br)Br)Br	Br	1.68E-08	2.24E-06
026040-51-7	O=C(OCC(CCCC)CC)c(c(c(c(c1Br)Br)Br)C(=O)OCC(CCCC)CC)c1Br	Br	1.71E-11	2.28E-09
026265-08-7	Oc(c(cc(c1)C(c(cc(c(O)c2Br)Br)c2)(C)C)Br)c1Br	Br	3.46E-11	4.61E-09

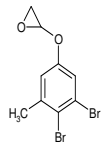
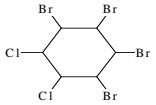
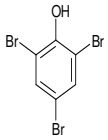
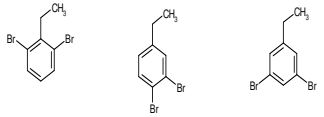
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
025357-79-3	438.54	-11.64	-1.20	10.44	3	0.499961866
025637-99-4	1.75	-5.15	7.74	12.89	6211	3.793161529
026040-51-7	0.49	-4.91	11.95	16.86	3	0.499961866
026265-08-7	3.62	-11.02	7.20	18.22	13552	4.132

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
025357-79-3	tetrabromophthalic acid; degradation product of several BFRs that are potential Penta BDE replacements	acid	N	N	Y
025637-99-4	Hexabromocyclododecane. Limited Great Lakes measurements. Possible penta BDE replacement. See also 3194556	neutral	Y	Y	
026040-51-7	Possible PentaBDE replacement; hydrolysis to diacid - LOGKOW 4.6 - looks very persistent. ; may be amendable to GC-MS	neutral	N	Y	
026265-08-7	Tetrabromobisphenol A containing product - with bisphenol A	phenol	Y	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
025357-79-3				N	0.5	0.5	10	10	
025637-99-4				Y	0.5				
026040-51-7		tetrabromophthalic acid	Y	N	10	10	10	10	10
026265-08-7	Y	TBBPA	Y	N	10	10	1	50	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
025357-79-3	–	Y	2.63E+05	Fish 96-hour LC_{50} (mg/L)	Marginal
025637-99-4		Y	9.17E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
026040-51-7	10	N	5.08E-04	Fish 96-hour LC_{50} (mg/L)	
026265-08-7	0.5	Y	5.00E-02	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
025357-79-3	25357793		Aliphatic amine
025637-99-4	25637994		Neutral Organics
026040-51-7	26040517		Neutral Organics
026265-08-7	26265087		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	030171-80-3	30171803	
Top 10 brominated	030554-72-4	30554724	
	030554-73-5	30554735	
	030812-87-4	30812874	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
030171-80-3	Brc2c(c(cc(c2)OCC1OC1)C)Br	Br	1.15E-04	1.53E-02
030554-72-4	BrC1C(C(C(C(C1Br)Br)Cl)Cl)Br	Br	8.38E-06	1.12E-03
030554-73-5	ClC1C(C(C(C(C1Cl)Cl)Br)Br)Br	Br	2.45E-05	3.27E-03
030812-87-4	Brc1c(cccc1CC)Br	Br	1.40E-02	1.87E+00

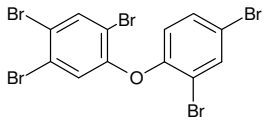
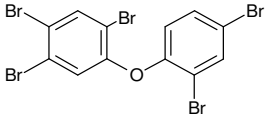
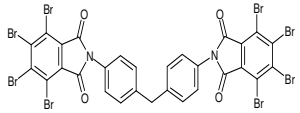
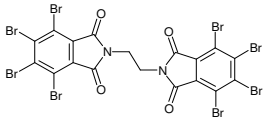
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
030171-80-3	0.60	-5.31	3.94	9.25	216	2.334453751
030554-72-4	16.36	-3.92	4.62	8.54	716	2.854791694
030554-73-5	16.86	-3.44	4.53	7.97	611	2.785899028
030812-87-4	5.41	-2.29	4.81	7.10	1011	3.004751156

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
030171-80-3	Analysable with other bromo/chlorobenzenes	neutral	N	Y	
030554-72-4	Analysable with other bromo/chlorobenzenes	neutral	N	Y	
030554-73-5	Tribromophenol	phenol	N	N	Y
030812-87-4	Analysable with other bromo/chlorobenzenes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
030171-80-3		Bromomethyl-phenol	Y	N		0.5		0.5	0.5
030554-72-4				N	0.5	0.5	0.5	0.5	
030554-73-5				N	0.5		1	10	10
030812-87-4				N	0.5	0.5	0.5		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
030171-80-3	–	Y	5.651	Fish 96-hour LC_{50} (mg/L)	
030554-72-4	–	Y	5.30E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
030554-73-5	–	Y	6.20E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
030812-87-4	–	Y	1.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
030171-80-3	30171803		Imides
030554-72-4	30554724		Neutral Organics
030554-73-5	30554735		Dinitrobenzenes
030812-87-4	30812874		Dinitrobenzenes

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	032534-81-9	32534819	
	032536-52-0	32536520	
	032588-74-2	32588742	
Top 10 brominated	032588-76-4	32588764	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
032534-81-9	Brc1cc(c(cc1Oc2c(cc(cc2)Br)Br)Br)Br	Br	2.44E-08	3.25E-06
032536-52-0	Brc1c(c(c(c(c1Br)Br)Br)Br)Oc2cc(c(cc2Br)Br)Br	Br	3.68E-11	4.91E-09
032588-74-2	O=C(N(c(ccc(c1)Cc(ccc(N(C(=O)c(c2c(c(c3Br)Br)Br)c3Br)C2=O)c4)c4)c1)C(=O)c5c(c(c(c6Br)Br)Br)Br)c56	Br	9.76E-27	1.30E-24
032588-76-4	O=C(N(C(=O)c1c(c(c(c2Br)Br)Br)Br)CCN(C(=O)c(c3c(c(c4Br)Br)Br)c4Br)C3(=O))c12	Br	2.54E-22	3.39E-20

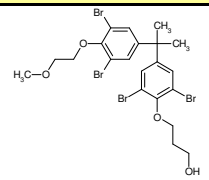
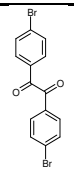
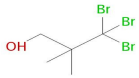
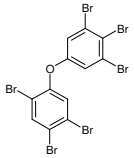
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
032534-81-9	19.44	-4.32	7.66	11.98	8058	3.906227263
032536-52-0	93.62	-5.51	10.33	15.84	3	0.499961866
032588-74-2	0.34	-19.12	11.16	30.28	3	0.499961866
032588-76-4	0.27	-18.83	9.80	28.63	10	0.978636948

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
032534-81-9	Penta BDE. Still in use but voluntarily withdrawn from production in 2005	neutral	Y	Y	
032536-52-0	Pentabromo BDE isomer. Now phased out of use in 2005. Another BFR Prod 1-10M all five years to 2002.	neutral	Y	Y	
032588-74-2	May yield tetrabromophthalic degradation products	neutral	N	Y	
032588-76-4	May yield tetrabromophthalic degradation products	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
032534-81-9				Y	10	10	10	50	50
032536-52-0				Y	10	50	50	10	50
032588-74-2		tetrabromophthalic acid	Y	N	0.5	0.5	0.5		
032588-76-4		tetrabromophthalic acid	Y	N	10	1	10	50	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
032534-81-9	–	Y	1.08E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
032536-52-0	–	N	6.63E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
032588-74-2	–	N	1.40E-05	Fish 96-hour LC_{50} (mg/L)	
032588-76-4	10	N	2.05E-04	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
032534-81-9	32534819		Neutral Organics
032536-52-0	32536520		Neutral Organics
032588-74-2	32588742		Neutral Organics
032588-76-4	32588764		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	033294-14-3	33294143	
	035578-47-3	35578473	
	036483-57-5	36483575	
	036483-60-0	36483600	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
033294-14-3	Brc2c(c(cc(c2)C(c1cc(c(c(c1)Br)OCCOC)Br)(C)C)Br)OCCCO	Br	7.43E-15	9.91E-13
035578-47-3	O=C(c(ccc(c1)Br)c1)C(=O)c(ccc(c2)Br)c2	Br	4.24E-07	5.65E-05
036483-57-5	BrC(C(CO)(C)C)(Br)Br	Br	2.87E-09	3.83E-07
036483-60-0	O(c(c(cc(c1)Br)Br)c1Br)CCOc(c(cc(c2)Br)Br)c2Br	Br	2.38E-10	3.17E-08

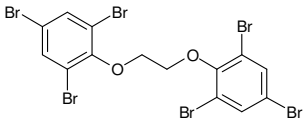
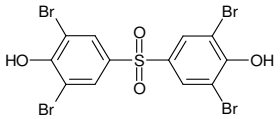
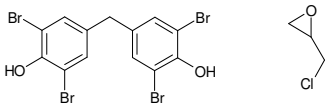
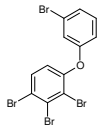
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
033294-14-3	0.32	-12.52	7.57	20.09	2407	3.38147609
035578-47-3	4.78	-8.30	5.34	13.64	2567	3.409425869
036483-57-5	30.44	-4.72	8.55	13.27	486	2.68690427
036483-60-0	0.72	-6.52	9.15	15.67	74	1.869407749

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
033294-14-3	Referred to as Oxirane, 2,2'-[(1-methylethylidene)bis [(2,6-dibromo-4,1-phenylene)oxy-methylene]]bis-, homopolymer; should degrade to TBBPA; maybe analysable by GC-MS	neutral	N	N	
035578-47-3	p,p'-Dibromobenzil Benzyl - may be chemical intermediate	neutral	N	Y?	
036483-57-5	Tribromoneopentyl Alcohol (Firemaster 550); should be amenable to GC analysis	neutral	N	Y	
036483-60-0	Benzene, 1,1 -oxybis-, hexabromo deriv.; part of Penta BDE product - now phase out but much in use chemical	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
033294-14-3		TBBPA	Y	N					1
035578-47-3				N				10	0.5
036483-57-5				N					
036483-60-0				Y	1		0.5		0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
033294-14-3	–	Y	1.54E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
035578-47-3		Y	5.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
036483-57-5		Y	6.01E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	
036483-60-0	–	N	8.94E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
033294-14-3	33294143		Neutral Organics
035578-47-3	35578473		Neutral Organics
036483-57-5	36483575		Neutral Organics
036483-60-0	36483600		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 brominated	037853-59-1	37853591	
	039635-79-5	39635795	
	040039-93-8	40039938	
	040088-47-9	40088479	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
037853-59-1	O(c(c(cc(c1)Br)Br)c1Br)CCOc(c(cc(c2)Br)Br)c2Br	Br	2.38E-10	3.17E-08
039635-79-5	O=S(=O)(c(cc(c(O)c1Br)Br)c1)c(cc(c(O)c2Br)Br)c2	Br	1.49E-13	1.99E-11
040039-93-8	Oc2c(Br)cc(Cc1cc(Br)c(O)c(Br)c1)cc2Br	Br	4.43E-11	5.91E-09
040088-47-9	Brc2c(c(ccc2Oc1cc(ccc1)Br)Br)Br	Br	2.41E-07	3.21E-05

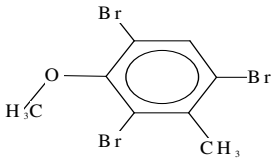
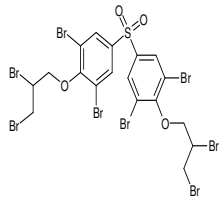
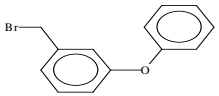
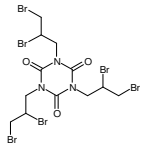
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
037853-59-1	0.72	-6.52	9.15	15.67	74	1.869407749
039635-79-5	21.08	-15.56	5.21	20.77	811	2.909074401
040039-93-8	33.27	-11.27	6.62	17.89	9854	3.993612558
040088-47-9	7.14	-3.92	6.77	10.69	32560	4.512684396

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
037853-59-1	Replacement for Penta and Decabromo BDEs. Limited measurements in the Great lakes region. Another BFR Prod 1-10M last two years	neutral	Y	Y	
039635-79-5	Phenol, 4,4'-sulfonylbis[2,6-dibromo-; Intermediate for production of flame retardants. May be analysable by LC-MS/MS ESI or after methylation by GC	phenol	N	N	Y
040039-93-8	Phenol, 4,4'-(1-methylethylidene)bis [2,6-dibromo-, polymer with (chloromethyl)oxirane; May be analysable by LC-MS/MS ESI or after methylation by GC	Phenol	N	N	Y
040088-47-9	Tetrabromodiphenyl ether - may be component in PentaBDE formulation	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
037853-59-1		Tribromophenol	Y	Y	50	50	50	10	10
039635-79-5	Y			N		0.5			
040039-93-8	Y			N	0.5	0.5		10	10
040088-47-9		OH-BDPE		Y	0.5		1		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
037853-59-1	10	N	1.70E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	
039635-79-5	–	Y	8.76E-01	Fish 96-hour LC_{50} (mg/L)	
040039-93-8	–	Y	1.08E-01	Fish 96-hour LC_{50} (mg/L)	
040088-47-9	–	Y	1.13E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
037853-59-1	37853591		Phenols
039635-79-5	39635795		Dinitrobenzenes
040039-93-8	40039938		Neutral Organics
040088-47-9	40088479		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	041424-36-6	41424366	
	042757-55-1	42757551	
	051632-16-7	51632167	
	052434-90-9	52434909	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
041424-36-6	Brc1c(C)c(Br)c(OC)c(Br)c1	Br	2.23E-04	2.97E-02
042757-55-1	BrCC(Br)COc1c(Br)cc(S(=O)(=O)c2cc(Br)c(OCC(Br)CBr)c(Br)c2)cc1Br	Br	7.67E-17	1.02E-14
051632-16-7	O(c(cccc1CBr)c1)c(cccc2)c2	Br	7.63E-05	1.02E-02
052434-90-9	N1(CC(Br)CBr)C(=O)N(CC(Br)CBr)C(=O)N(CC(Br)CBr)C1(=O)	Br	1.18E-15	1.57E-13

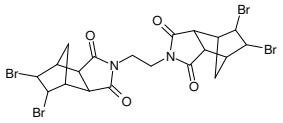
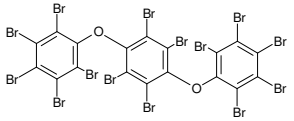
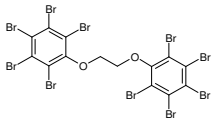
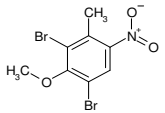
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
041424-36-6	7.22	-3.04	5.29	8.33	2367	3.374198258
042757-55-1	1.42	-12.31	9.52	21.83	23	1.357363031
051632-16-7	1.04	-3.21	4.94	8.15	1270	3.103803721
052434-90-9	1.63	-16.31	7.37	23.68	19890	4.298634783

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
041424-36-6	Benzene, 1,3,5-tribromo-2-methoxy-4-methyl-; Analysable with other bromo/chlorobenzenes	neutral	N	Y	
042757-55-1	Derivative of 39635-79-5; should be analysable by GC-MS	neutral	N	Y	
051632-16-7	Benzyl bromide will hydrolyze - chemical intermediate?	neutral	N	Y	
052434-90-9	Should be analysable by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
041424-36-6				N					
042757-55-1		bis-phenol	Y	N	0.5				
051632-16-7		OH-BDPE		Y	10	10	10	10	10
052434-90-9				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
041424-36-6	–	Y	6.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
042757-55-1	–	N	8.22E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	
051632-16-7		Y	1.59E-01	Fish 96-hour LC_{50} (mg/L)	
052434-90-9	–	Y	2.10E-02	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
041424-36-6	41424366		Dinitrobenzenes
042757-55-1	42757551		Dinitrobenzenes
051632-16-7	51632167		Neutral Organics
052434-90-9	52434909		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	052907-07-0	52907070	
	058965-66-5	58965665	
	61262-53-1	61262531	
	061262-53-1	62265990	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
052907-07-0	O=C4(N(CCN2(C(=O)C1(C3(C(Br)C(Br)C(C1C2(=O))C3))))C(=O)C5(C6(C(Br)C(Br)C(C45)C6)))	Br	6.26E-19	8.35E-17
058965-66-5	Brc2(c(Br)c(Oc1(c(Br)c(Br)c(Br)c(Br)c1Br))c(Br)c(Br)c2Oc3(c(Br)c(Br)c(Br)c(Br)c3Br))	Br	3.68E-20	4.91E-18
61262-53-1	O(c(c(c(c(c1Br)Br)Br)Br)c1Br)CCOc(c(c(c(c2Br)Br)Br)Br)c2Br	Br	3.22E-14	4.29E-12
061262-53-1	O=N(=O)c(c(c(c(OC)c1Br)Br)C)c1	Br	0.0000273	0.003639701

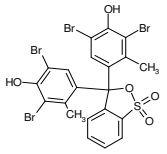
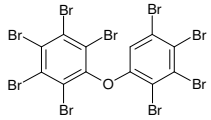
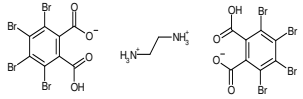
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
052907-07-0	0.18	-18.79	1.96	20.75	6	0.812311609
058965-66-5	195.93	-9.57	16.89	26.46	3	0.499961866
61262-53-1	0.74	-9.12	12.71	21.83	3	0.499961866
061262-53-1	123.7580279	-5.046148095	4.22	5.871860707	353.6	2.549

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
052907-07-0	Should be analysable by GC-MS	neutral	N	Y	
058965-66-5	Use may be simsilar to deacbromoBDE. 14 Br atoms, P - probably not B unless it breakdown	neutral	N	Y	
61262-53-1	Possible decaBDE replacement. Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis [2,3,4,5,6-pentabromo-. May yield pentabromophenol on degradation	neutral	N	Y	
061262-53-1	P - two Br, one Nitro but no production DSL	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
052907-07-0				N		1	0.5		
058965-66-5		Pentabromophenol	Y	N		1	1	10	10
61262-53-1		Pentabromophenol	Y	N	1				
061262-53-1				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
052907-07-0	–	Y	3.92E+02	Fish 96-hour LC_{50} (mg/L)	
058965-66-5	–	N	7.13E-17	Mysid Shrimp 96-hour LC_{50} (mg/L)	
61262-53-1	–	N	8.79E-12	Mysid Shrimp 96-hour LC_{50} (mg/L)	
061262-53-1			0.117	Mysid Shrimp 96-hour LC_{50} (mg/L)	High-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
052907-07-0	52907070		Neutral Organics
058965-66-5	58965665		Neutral Organics
61262-53-1	61262531		Esters + Phenols
061262-53-1	62265990	airbreather	Anilines (amino-meta)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	62625-32-5	62625325	
	062625-32-5	63936561	
	66046-78-4	66046784	
	066046-78-4	68758758	No structure

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
62625-32-5	c12S(=O)(=O)OC(c4c(C)c(Br)c(O)c(Br)c4)(c3c(C)c(Br)c(O[Na])c(Br)c3)c1ccccc2	Br	3.16E-24	4.21E-22
062625-32-5	BrC2(C(OC1(=C(Br)C(Br)=C(Br)C(Br)=C1))=C(Br)C(Br)=C(Br)C=2Br)	Br	4.03E-12	5.37E-10
66046-78-4	c1(c(c(c(c(c1Br)Br)Br)Br)C(=O)ON(H)(H)(H)CCN(H)(H)(H)OC(=O)c1(c(c(c(c(c1Br)Br)Br)Br)C(=O)O))C(=O)O	Br	4.96E-28	6.61E-26
066046-78-4	No structure	Br		

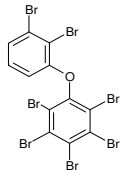
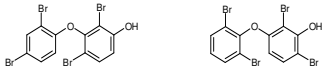
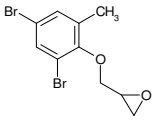
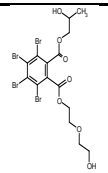
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
62625-32-5	2.34	-16.33	5.18	21.51	1699	3.230193379
062625-32-5	161.01	-5.91	11.22	17.13	3	0.499961866
66046-78-4	0.48	-33.77	7.37	41.14	10	1
066046-78-4						

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
62625-32-5	TBBPA related. May degrade to PTBBA	phenol	N	N	Y?
062625-32-5	Nonabromo BDE. Component of deac BDE formulation. Benzene, pentabromo(tetrabromophenoxy)-	neutral	Y	Y	
66046-78-4	See also 25357-79-3. Essentially the same product. 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetra-bromo□, compd. with 1,2-ethanediamine (2:1)	acid	N	N	Y
066046-78-4	Google search revealed it was a tetrabromo-, polymer with (chloromethyl)oxirane and 4,4'- (1-methylethylidene) with tetrabromobisphenolA	acid	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
62625-32-5	Y			N					
062625-32-5		OH-BDPE		Y	1	1	1		0.5
66046-78-4		tetrabromophthalic acid	Y	N	10	10	10		
066046-78-4		TBBPA?	Y	N	50				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
62625-32-5		Y	0.406	Mysid Shrimp 96-hour LC_{50} (mg/L)	
062625-32-5	–	N	5.62E-10	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
66046-78-4	–	Y	4.24E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
066046-78-4		Y	NA		Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
62625-32-5	62625325		Peroxy Esters
062625-32-5	63936561		amine
66046-78-4	66046784		Phenols
066046-78-4	68758758		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068928-80-3	68928803	
	069882-11-7	69882117	
	075150-13-9	75150139	
	077098-07-8	77098078	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068928-80-3	Brc2c(c(c(c(c2Br)Br)Br)Br)Oc1c(c(ccc1)Br)Br	Br	3.29E-10	4.39E-08
069882-11-7	Oc2ccc(Br)c(Oc1ccc(Br)cc1Br)c2Br	Br	3.19E-09	4.25E-07
075150-13-9	Cc1cc(cc(c1OCC2CO2)Br)Br	Br	1.15E-04	1.53E-02
077098-07-8	O=C(c1c(c(c(c(c1C(=O)OCCOCCO)Br)Br)Br)Br)OCC(C)O	Br	2.37E-14	3.16E-12

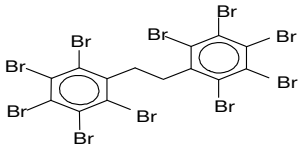
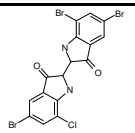
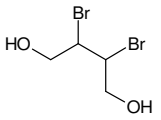
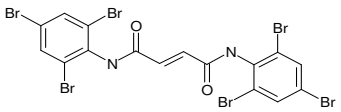
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
068928-80-3	35.51	-5.11	9.44	14.55	29	1.467608106
069882-11-7	27.87	-7.91	6.29	14.20	5532	3.742882171
075150-13-9	1.14	-5.31	3.94	9.25	216	2.334453751
077098-07-8	0.35	-13.95	3.83	17.78	39	1.59571662

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068928-80-3	Heptabromo BDE. Component of "Octa BDE" formulation. Benzene, 1,1 -oxybis-, heptabromo deriv. No phase out although product remains in existing end use items	neutral	Y	Y	
069882-11-7	May be intermediate used to make polymer. Phenol, 2,4(or 2,6)-dibromo-, homopolymer. Sold as "Poly(2,6-dibromophenylene oxide)". Residual hydroxy brominated BDE has been analysed in Great Lakes waters	Phenol	N	N	Y
075150-13-9	Oxirane, [(2,4-dibromo-6-methylphenoxy)-methyl]-; Should be analysable by GC-MS	neutral	N	Y	
077098-07-8	Possible PentaBDE replacement; hydrolysis to diacid. - similar to 026040-51-May not be analysable by GC due alcohol groups	neutral	N	N	Y?

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068928-80-3		OH-BDPE		Y	1	0.5	1	0.5	0.5
069882-11-7		OH-BDPE	Y	Y	0.5				
075150-13-9		dibromo-methyl-phenol	Y	N				0.5	
077098-07-8	Y?	tetrabromophthalic acid	Y	N		10	10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068928-80-3	–	N	7.74E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
069882-11-7	0.5	Y	1.68E-01	Fish 96-hour LC_{50} (mg/L)	
075150-13-9	–	Y	5.651	Fish 96-hour LC_{50} (mg/L)	
077098-07-8	10	Y	9.97E+00	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068928-80-3	68928803		Esters
069882-11-7	69882117		Neutral Organics
075150-13-9	75150139		Neutral Organics
077098-07-8	77098078		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 brominated	84852-53-9	84852539	
	085702-64-3	85702643	
	090801-18-6	90801186	
	092484-07-6	92484076	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
84852-53-9	Brc2c(Br)c(Br)c(CCc1c(Br)c(Br)c(Br)c(Br)c1Br)c(Br)c2Br	Br		2.53313E-11
085702-64-3	O=C1C(=C2Nc3c(cc(cc3Cl)Br)C2(=O))Nc4c1cc(cc4Br)Br	Br	2.77E-12	3.69303E-10
090801-18-6	OCC(C(CO)Br)Br	Br	6.53E-05	8.71E-03
092484-07-6	O=C(Nc1c(cc(cc1Br)Br)Br)C=CC(=O)Nc2c(cc(cc2Br)Br)Br	Br	1.46E-16	1.95E-14

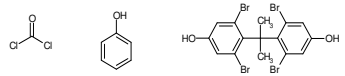
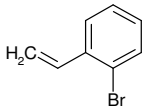
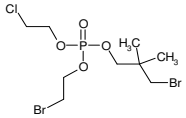
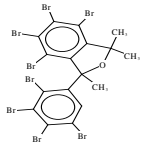
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
84852-53-9	4.50	-5.920223446	13.64	19.56022345	3.16	
085702-64-3	21.46193083	-13.01750291	6.43	16.05321553	2570	3.410
090801-18-6	2.74	-6.90	0.32	7.22	3	0.499961866
092484-07-6	1.15	-14.35	5.76	20.11	5422	3.734159513

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
84852-53-9	1,1'-(Ethane-1,2-diyl)bis(pentabromobenzene). may be just used in Europe. No IUR or DSL listing. Reported in GL herring gull eggs and in biota from the Baltic Sea (Kierkegaard et al EST 2004). LPV chemical in Europe but not listed on EPA IUR	neutral	Y	Y	
085702-64-3	Possible P, B	neutral	N	Y	
090801-18-6	1,4-Butanediol, 2,3-dibromo-	neutral	N	N	Y?
092484-07-6	Potential pentaBDE replacemenet. May degrade to tribromoaniline. 2-Butenediamide, N,N'-bis(2,4,6-tribromophenyl)-, (2E)-	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
84852-53-9		Y	Y	N					No Reports (>3
085702-64-3				N			0.5	0.5	0.5
090801-18-6				N		1	0.5		
092484-07-6		tribromoaniline	Y	N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
84852-53-9	No Reports		5.80E-13	Mysid Shrimp 96-hour LC50 (mg/L)	
085702-64-3	–	Y	2.00E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
090801-18-6		Y	280.827	Fish 96-hour LC_{50} (mg/L)	
092484-07-6	–	Y	1.218	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
84852-53-9	84852539		Neutral Organics
085702-64-3	85702643	MPV	Neutral Organics
090801-18-6	90801186		Neutral Organics
092484-07-6	92484076		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	094334-64-2	94334642	
	125904-11-2	125904112	
	125997-20-8	125997208	
Top 10 brominated	155613-93-7	155613937	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
094334-64-2	CC(C)(c1c(Br)cc(O)cc1Br)c2c(Br)cc(O)cc2Br	Br	1.76E-11	2.35E-09
125904-11-2	C=Cc1ccccc1Br	Br	2.27E-01	3.03E+01
125997-20-8	O=P(OCCBr)(OCCCl)OCC(CBr)(C)C	Br	0.00000439	0.000585285
155613-93-7	CC3(C)OC(C)(c1cc(Br)c(Br)c(Br)c1Br)c2c(Br)c(Br)c(Br)c(Br)c23	Br	1.23E-12	1.64E-10

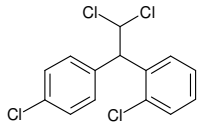
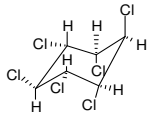
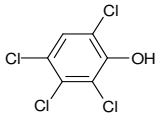
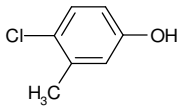
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
094334-64-2	3.97	-11.02	7.20	18.22	13550	4.131939295
125904-11-2	0.23	-1.35	3.78	5.13	164	2.214578954
125997-20-8	3.156475195	-6.583750097	3.17	6.359462709	9.219	0.965
155613-93-7	6.20	-6.91	11.80	18.71	1	

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
094334-64-2	Carbonic dichloride, polymer with 4,4'-(1-methylethylidene)bis [2,6-dibromophenol] and phenol tetrabromobisphenol related	phenol	Y	N	Y
125904-11-2	Benzene, ethenyl-, ar-bromo derivs.; Should be analysable by GC-MS	neutral	N	Y	
125997-20-8	P? phosphate esters biodeg, high production	neutral	N	Y	
155613-93-7	Octabromo-1,1,3-trimethyl-3-phenyl indan; should be analysable by GC MS with PBDEs	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
094334-64-2		TBBPA	Y	N	0.5				
125904-11-2				N		10	10	10	10
125997-20-8		phosphate	Y	N		10	10	10	
155613-93-7				N				10	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
094334-64-2	–	Y	5.00E-02	Fish 96-hour LC_{50} (mg/L)	
125904-11-2	50	Y	2.33E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
125997-20-8	–	Y	8.1	Fish 96-hour LC_{50} (mg/L)	Low-moderate
155613-93-7		N	1.05E-10	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
094334-64-2	94334642		Neutral Organics
125904-11-2	125904112		Neutral Organics
125997-20-8	125997208	airbreather	Neutral Organics
155613-93-7	155613937		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000053-19-0	53190	
	000058-89-9	58899	
	000058-90-2	58902	
	000059-50-7	59507	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000053-19-0	ClC(Cl)C(c1ccc(Cl)cc1)c2ccccc2Cl	Cl	1.69E-05	2.25E-03
000058-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	Cl	0.000506	0.067461118
000058-90-2	Oc(c(cc(c1Cl)Cl)Cl)c1Cl	Cl	0.000489	0.065194638
000059-50-7	Oc(ccc(c1C)Cl)c1	Cl	0.0103	1.373220395

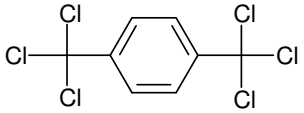
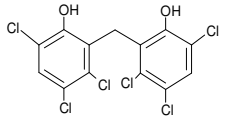
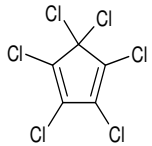
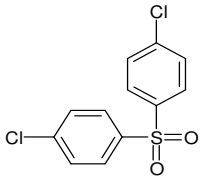
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000053-19-0	2.46	-2.75	5.87	8.62	6645	3.822494985
000058-89-9	223.9172944	-1.980330811	4.26	2.846043422	307.5	2.488
000058-90-2	464.3511522	-5.160684071	4.09	5.856396683	212.1	2.327
000059-50-7	4.998716407	-4.727705298	2.7	4.03341791	48.64	1.687

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000053-19-0	DDD related	neutral	Y	Y	
000058-89-9	HCH - see what isomer	neutral	Y	Y	
000058-90-2		phenol	Y	N	Y
000059-50-7		phenol	Y	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000053-19-0				Y					
000058-89-9				Y				0.5	
000058-90-2				Y					
000059-50-7				N	0.5	0.5	0.5	1	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000053-19-0		Y	9.95E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000058-89-9		Y	0.093	Mysid Shrimp 96-hour LC_{50} (mg/L)	moderate
000058-90-2		Y	1.757	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000059-50-7		Y	7.76	Fish 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
000053-19-0	53190		Phenols
000058-89-9	58899	airbreather	Neutral Organics
000058-90-2	58902	airbreather	Phenols
000059-50-7	59507	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000068-36-0	68360	
	000070-30-4	70304	
5. Top 10 chlorinated	000077-47-4	77474	
5. Top 10 chlorinated	000080-07-9	80079	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000068-36-0	c(ccc(c1)C(Cl)(Cl)Cl)(c1)C(Cl)(Cl)Cl	Cl	5.13E-04	6.84E-02
000070-30-4	Oc(c(c(c(c1)Cl)Cl)Cc(c(c(cc2Cl)Cl)Cl)c2O)c1Cl	Cl	8.31E-11	1.11E-08
000077-47-4	C(=C(C(=C1Cl)Cl)Cl)(C1(Cl)Cl)Cl	Cl	4.88E-02	6.51E+00
000080-07-9	O=S(=O)(c(ccc(c1)Cl)c1)c(ccc(c2)Cl)c2	cl	0.000000809	0.000107858

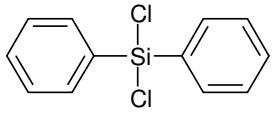
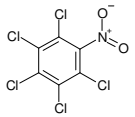
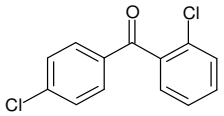
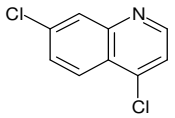
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000068-36-0	222.46	-3.29	5.80	9.09	720	2.857392811
000070-30-4	4.91	-10.45	6.92	17.37	4680	3.670245853
000077-47-4	26.99	-1.06	4.63	5.69	1516	3.180699201
000080-07-9	218.8586343	-5.251850209	3.9	5.75756282	199.5	2.300

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000068-36-0	Hexachloroxylene (Benzene, 1,4-bis[trichloromethyl]-). Two benzoyl chlorides - hydrolyze fast?	neutral	N	Y	
000070-30-4	Hexachlorophene. May be analysable with other chlorophenol related compounds and triclosan	phenol	N	N	Y
000077-47-4	analog search maleic anhydride analog - 1M - 10M, acid varies 2002 500K-1M, 2-EH ester of acid 10K-500K, Dichlorane Plus 1M-10M, Heptachlorocyclopentene - 1M - 10M but no derivatives - used in polymers??	neutral	N	Y	
000080-07-9	bis-2chlorophenyl sulfone has been reported in wildlife by Olsso	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000068-36-0				N	10	10	10		
000070-30-4	Y			N					
000077-47-4				N	50	50	50	50	50
000080-07-9				N	10	10	50	50	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000068-36-0		Y	2.12E-01	Fish 14-day LC_{50} (mg/L)	
000070-30-4		Y	5.60E-02	Fish 96-hour LC_{50} (mg/L)	Low
000077-47-4		Y	0.346	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000080-07-9		Y	0.259	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000068-36-0	68360		Esters + Phenols
000070-30-4	70304		Phenols
000077-47-4	77474		amine
000080-07-9	80079	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000080-10-4	80104	
	000082-68-8	82688	
	000085-29-0	85290	
	000086-98-6	86986	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000080-10-4	Cl[Si](c1ccccc1)(c2ccccc2)Cl	Cl	6.05E-04	8.07E-02
000082-68-8	O=N(=O)c(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl	Cl	2.72E-05	3.63E-03
000085-29-0	O=C(c(ccc(c1)Cl)c1)c(c(ccc2)Cl)c2	cl	0.0000814	0.010852441
000086-98-6	n(c(c(c(c1)Cl)ccc2Cl)c2)c1	cl	0.000608	0.08106

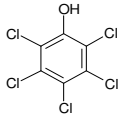
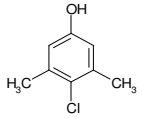
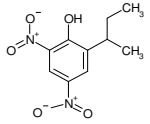
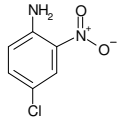
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000080-10-4	2.74	-2.54	5.06	7.60	1564	3.194236749
000082-68-8	1479.39	-3.71	5.03	8.74	746	2.87279704
000085-29-0	51.32883695	-4.359186998	4.44	5.40489961	75.13	1.876
000086-98-6	53.87574931	-4.811078976	3.43	4.846791588	111.9	2.049

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000080-10-4	May hydrolyse rapidly in ambient air	neutral	N	N	
000082-68-8	Pentachloronitrobenzene currently on analytical lists	neutral	Y	Y	
000085-29-0		neutral	N	Y	
000086-98-6		neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000080-10-4		Silanol	Y?	N	10	10	10	1	0.5
000082-68-8				Y			10		
000085-29-0				N	0.5				
000086-98-6				N	0.5	0.5	0.5		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000080-10-4		N	8.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000082-68-8		Y	3.20E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
000085-29-0		Y	0.048	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000086-98-6		Y	0.691	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000080-10-4	80104		Neutral Organics
000082-68-8	82688		Neutral Organics
000085-29-0	85290	airbreather	Esters
000086-98-6	86986	airbreather	Vinyl/Allyl Ethers

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000087-86-5	87865	
	000088-04-0	88040	
	000088-85-7	88857	
	000089-63-4	89634	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000087-86-5	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl	cl	0.0000108	0.001439882
000088-04-0	Oc(cc(c(c1C)Cl)C)c1	cl	0.0018	0.239980263
000088-85-7	N(=O)(=O)c(cc(N(=O)(=O))c(O)c1C(CC)C)c1	Cl	7.44E-05	9.92E-03
000089-63-4	N(=O)(=O)c(c(N)ccc1Cl)c1	cl	0.000266	0.03546375

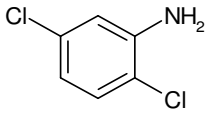
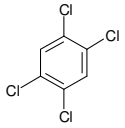
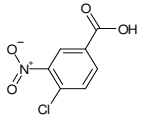
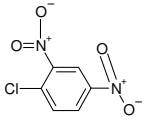
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000087-86-5	233.1751512	-5.291660763	4.74	6.637373375	695.7	2.842
000088-04-0	1.923631592	-4.684420259	3.25	4.540132871	65.75	1.818
000088-85-7	2.65	-5.54	3.67	9.21	110	2.041392685
000089-63-4	32.67769215	-5.302210945	2.66	4.567923557	24.8	1.394

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000087-86-5		phenol	Y	N	Y
000088-04-0	disinfectant; Chloroxylenol	phenol	N	N	Y
000088-85-7	current use pesticide, Dinoseb	phenol	Y	N	Y
000089-63-4		neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000087-86-5				Y					
000088-04-0				N	0.5	0.5		0.5	
000088-85-7				N	10	10	10	10	10
000089-63-4				N	0.5	0.5	1	1	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000087-86-5		Y	0.803	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000088-04-0		Y	3.907	Fish 96-hour LC_{50} (mg/L)	Marginal
000088-85-7		Y	1.28E+00	Fish 96-hour LC_{50} (mg/L)	Low
000089-63-4		Y	11.27	Fish 96-hour LC_{50} (mg/L)	High-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000087-86-5	87865	airbreather	Phenols
000088-04-0	88040	airbreather	Neutral Organics
000088-85-7	88857		Neutral Organics
000089-63-4	89634	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000095-82-9	95829	
	000095-94-3	95943	
	000096-99-1	96991	
	000097-00-7	97007	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000095-82-9	Nc(c(ccc1Cl)Cl)c1	cl	0.0149	1.986503289
000095-94-3	c(c(cc(c1Cl)Cl)Cl)(c1)Cl	Cl	2.47E-03	3.29E-01
000096-99-1	O=C(O)c(ccc(c1N(=O)=O)Cl)c1	cl	0.00000432	0.000575953
000097-00-7	N(=O)(=O)c(ccc(c1N(=O)(=O))Cl)c1	Cl	4.84E-04	6.45E-02

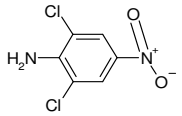
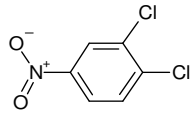
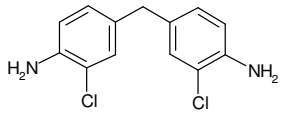
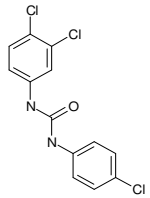
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000095-82-9	5.805662666	-4.367381477	2.37	3.343094089	26.15	1.417
000095-94-3	130.04	-1.18	4.57	5.75	746	2.87279704
000096-99-1	219.9951823	-7.887511514	2.34	6.833224125	3.162	0.500
000097-00-7	499.35	-5.59	2.27	7.86	9	0.970904498

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000095-82-9	P? two Cls - should be some experimental - herbicide metabolite	amine	Y	Y	
000095-94-3	chlorobenzene; legacy chemical already on analyte lists	neutral	Y	Y	
000096-99-1	P? Nitro and Cl	neutral	N	N	Y
000097-00-7	should be very persistent but not bioaccumulative	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000095-82-9				N	0.5	0.5	0.5	0.5	0.5
000095-94-3				Y	10	10	10	10	
000096-99-1				N		0.5	0.5	0.5	
000097-00-7				N	10	10	10	50	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000095-82-9		Y	15.123	Fish 96-hour LC_{50} (mg/L)	moderate
000095-94-3		Y	2.30E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
000096-99-1		Y	616.121	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000097-00-7		Y	1.58E+00	Fish 96-hour LC_{50} (mg/L)	High-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000095-82-9	95829	airbreather	Neutral Organics
000095-94-3	95943		Phenols
000096-99-1	96991	airbreather	Neutral Organics
000097-00-7	97007		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000099-30-9	99309	
	000099-54-7	99547	
	000101-14-4	101144	
5. Top 10 chlorinated	000101-20-2	101202	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000099-30-9	O=N(=O)c(cc(c(N)c1Cl)Cl)c1	cl	0.000012	0.001599868
000099-54-7	N(=O)(=O)c(ccc(c1Cl)Cl)c1	cl	0.0138	1.839848684
000101-14-4	Nc(c(cc(c1)Cc(ccc(N)c2Cl)c2)Cl)c1	Cl	3.93E-06	5.24E-04
000101-20-2	O=C(Nc(ccc(c1)Cl)c1)Nc(ccc(c2Cl)Cl)c2	Cl	3.61E-09	4.81E-07

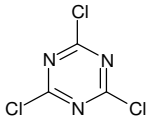
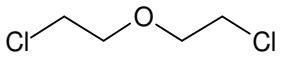
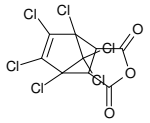
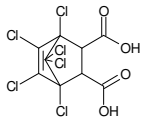
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000099-30-9	929.2737928	-6.77367356	2.76	6.139386172	28.58	1.456
000099-54-7	2564.647133	-3.320384914	3.1	3.026097526	50.4	1.702
000101-14-4	0.14	-8.87	3.47	12.34	205	2.310693312
000101-20-2	0.50	-8.73	4.90	13.63	1187	3.074450719

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000099-30-9	P - 2 Cl, Nitro	amine	N	Y	
000099-54-7	P - 2 Cls, Nitro	neutral	N	Y	
000101-14-4	4,4'-Methylene bis(2-chloroaniline. Persistent exp data (DSL) - probably susceptible to photolysis - 4,4'-Methylene-bis(2-chloroaniline)/ (MOCA). amine used as a curing agent for isocyanate-containing polymers.	neutral	N	Y	
000101-20-2	Triclocarban. Microbicide. Looks very persistent. Some environmental measurements in the Great Lakes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000099-30-9				N	1	10	0.5	0.5	0.5
000099-54-7				N	50	50			
000101-14-4				N	10	10	10	10	10
000101-20-2				N	0.5	10	10	1	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000099-30-9		Y	12.029	Fish 96-hour LC_{50} (mg/L)	High-moderate
000099-54-7		Y	7.256	Mysid Shrimp 96-hour LC_{50} (mg/L)	moderate
000101-14-4		Y	6.627	Fish 96-hour LC_{50} (mg/L)	High-moderate
000101-20-2		Y	1.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000099-30-9	99309	airbreather	Neutral Organics
000099-54-7	99547	airbreather	Neutral Organics
000101-14-4	101144		Neutral Organics
000101-20-2	101202		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000108-77-0	108770	
	000111-44-4	111444	
	000115-27-5	115275	
	000115-28-6	115286	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000108-77-0	n(c(nc(n1)Cl)Cl)c1Cl	Cl	2.36E-02	3.15E+00
000111-44-4	O(CCCl)CCCl	Cl	1.04E+00	1.39E+02
000115-27-5	O=C(OC(=O)C1C(C(=C(C23Cl)Cl)Cl)(C3(Cl)Cl)Cl)C12	Cl	6.46E-07	8.61E-05
000115-28-6	O=C(O)C(C(C(=C(C12Cl)Cl)Cl)(C1(Cl)Cl)Cl)C2C(=O)O	Cl	1.44E-08	1.92E-06

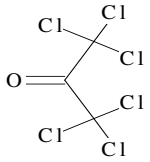
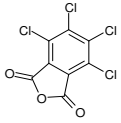
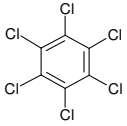
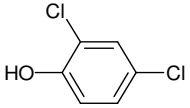
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000108-77-0	2867.56	-4.70	1.73	6.43	2	0.314288661
000111-44-4	3.39	-2.11	1.56	3.67	2	0.293362555
000115-27-5	1.95	-5.44	4.37	9.81	460	2.66238002
000115-28-6	320.20	4.98	3.14	-1.84	1	-0.301029996

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000108-77-0	several triazines (persistent) producted in 100-500M. Probably used mostly as a chemical intermediate for triazine herbicides	neutral	N	Y	
000111-44-4	This is a compound that used to be detected a lot because it was the intermediate and by-product from chlorohydrin synthesis of ethylene oxide. Still produced in 1-10M.for all 5 years.	neutral	N	Y	
000115-27-5	Chlorendic Anhydride. May be from hexachlorocyclopentadiene Prod 1-10M - will hydrolyze to the acid (000115-28-6). Degradation product Chlorendic acid	neutral	N	Y?	
000115-28-6	May be amenable to GC-MS after derivatization. See also the anhydride 115-27-5	acid	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000108-77-0				N	50	50	100	50	500
000111-44-4				N	10	10	10	10	10
000115-27-5		Chlorendic acid	Y	N	10	10	10	10	10
000115-28-6				N	1	10			1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000108-77-0		Y	167.185	Fish 96-hour LC_{50} (mg/L)	
000111-44-4		Y	73.377	Fish 96-hour LC_{50} (mg/L)	Low
000115-27-5		Y	2.14E-01	Fish 96-hour LC_{50} (mg/L)	
000115-28-6		Y	1.44E+01	Fish 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
000108-77-0	108770		Neutral Organics
000111-44-4	111444		Phenols
000115-27-5	115275		Esters + Esters (phosphate)
000115-28-6	115286		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000116-16-5	116165	
	000117-08-8	117088	
	000118-74-1	118741	
	000120-83-2	120832	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000116-16-5	O=C(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl	Cl	3.10E-01	4.13E+01
000117-08-8	O=C(OC(=O)c1c(c(c(c2Cl)Cl)Cl)Cl)c12	Cl	5.16E-07	6.88E-05
000118-74-1	c(c(c(c(c1Cl)Cl)Cl)Cl)(c1Cl)Cl	Cl	3.05E-06	4.07E-04
000120-83-2	Oc(c(cc(c1)Cl)Cl)c1	cl	0.0657	8.759279605

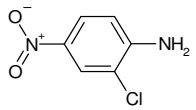
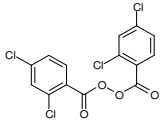
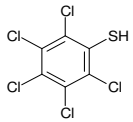
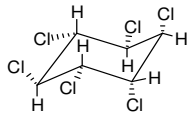
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000116-16-5		-11.91	2.48	14.39	16	1.206556044
000117-08-8	338.37	-4.11	4.65	8.76	755	2.878061981
000118-74-1	633.27	-1.44	5.86	7.30	5153	3.712060142
000120-83-2	43.05870697	-4.900020059	2.8	4.305732671	18.04	1.256

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000116-16-5	Hexachloroacetone. Not HPV looks very persistent e.g. ground water.	neutral	N	Y	
000117-08-8	hydrolyzes to diacid. Prod 1-10M 14 with related structures - esters, imides, amides, about half do not have production data.	acid	N	N	Y
000118-74-1	Hexachlorobenzene; already on POPs list	neutral	Y	Y	
000120-83-2	Not very P - 2,4-D metabolite, DSL P??	phenol	Y	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000116-16-5				N	0.5	0.5			0.5
000117-08-8		Tetrachlorophthalic acid	Y	N	10	10	10	10	10
000118-74-1		Tetrachlorophthalic acid	Y	Y				0.5	0.5
000120-83-2				N	50	50	50	100	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000116-16-5		Y	1.42E+01	Mysid Shrimp 96-hour LC_{50} (mg/L)	High-moderate
000117-08-8		Y	3.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000118-74-1		Y	1.32E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
000120-83-2		Y	6.288	Fish 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
000116-16-5	116165		Neutral Organics
000117-08-8	117088		Phenols
000118-74-1	118741		Phenols
000120-83-2	120832	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000121-87-9	121879	
	000133-14-2	133142	
5. Top 10 chlorinated	000133-49-3	133493	
	000319-84-6	319846	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000121-87-9	O=N(=O)c(ccc(N)c1Cl)c1	cl	0.00034	0.045329605
000133-14-2	O=C(OOC(=O)c(c(cc(c1)Cl)Cl)c1)c(c(cc(c2)Cl)Cl)c2	Cl	1.06E-06	1.41E-04
000133-49-3	Sc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl	Cl	1.87E-04	2.49E-02
000319-84-6	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	cl	0.000506	0.067461118

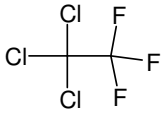
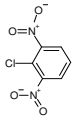
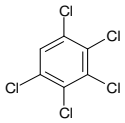
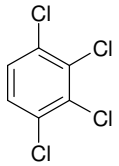
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000121-87-9	32.67769215	-6.642715581	2.12	5.368428192	8.497	0.929
000133-14-2	6.08	-4.36	6.01	10.37	8478	3.928293412
000133-49-3	76.72	-2.32	5.91	8.23	7066	3.849173633
000319-84-6	223.9172944	-1.980330811	4.26	2.846043422	307.5	2.488

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000121-87-9	P - Cl, nitro	neutral	N	Y	
000133-14-2	May hydrolyse to chlorobenzoic acids	acid	N	N	
000133-49-3	May be analysed by GC-MS. Not HPV	phenol	N	Y	
000319-84-6	HCH - which isomer?	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000121-87-9					0.5	0.5	0.5	0.5	
000133-14-2		dichlorobenzoate	Y	N	0.5	0.5	0.5	0.5	0.5
000133-49-3				N	1	1	1	0.5	0.5
000319-84-6				Y		0.5	0.5		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000121-87-9		Y	21.714	Fish 96-hour LC_{50} (mg/L)	moderate
000133-14-2		Y	0.051	Fish 96-hour LC_{50} (mg/L)	
000133-49-3		Y	0.058	Fish 96-hour LC_{50} (mg/L)	Moderate
000319-84-6		Y	2.308	Fish 96-hour LC_{50} (mg/L)	moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000121-87-9	121879	airbreather	Neutral Organics
000133-14-2	133142		amine
000133-49-3	133493		Neutral Organics
000319-84-6	319846	airbreather	Peroxy Acids

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000354-58-5	354585	
	000606-21-3	606213	
	000608-93-5	608935	
	000634-66-2	634662	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000354-58-5	FC(F)(F)C(Cl)(Cl)Cl	Cl	3.41E+02	4.55E+04
000606-21-3	O=N(=O)c(c(c(N(=O)=O)cc1)Cl)c1	Cl	0.000217	0.028930954
000608-93-5	c(c(c(c(c1Cl)Cl)Cl)Cl)(c1)Cl	Cl	1.71E-03	2.28E-01
000634-66-2	c(c(c(c(c1)Cl)Cl)Cl)(c1)Cl	Cl	1.35E-02	1.80E+00

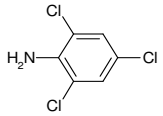
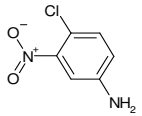
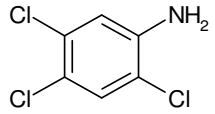
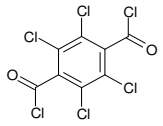
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000354-58-5		1.04	3.09	2.05	48	1.683047038
000606-21-3	5992.557843	-5.594780391	2.27	4.470493003	11.22	1.050
000608-93-5	184.86	-1.31	5.22	6.53	1909	3.280805928
000634-66-2	130.04	-1.18	4.57	5.75	695	2.841984805

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000354-58-5	1,1,1-trifluorotrichloroethane. Fully halogenated GWP and ODP 100-500M in 1998 & 2002 - large production several other; atmospheric measurements	neutral	Y	Y	
000606-21-3	P but probably no B	neutral	Y	Y	
000608-93-5	pentachlorobenzene; legacy POP related	neutral	Y	Y	
000634-66-2	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000354-58-5				N	10	10	50	500	500
000606-21-3				N	0.5	0.5	1	1	
000608-93-5				Y					
000634-66-2				Y	10	10	10	1	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000354-58-5		Y	1.74E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000606-21-3		Y	3.983	Fish 96-hour LC_{50} (mg/L)	moderate
000608-93-5		Y	6.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
000634-66-2		Y	2.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000354-58-5	354585		Acid Chloride/Halide
000606-21-3	606213	airbreather	Aliphatic amine
000608-93-5	608935		Esters
000634-66-2	634662		Hydrazines

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000634-93-5	634935	
	000635-22-3	635223	
	000636-30-6	636306	
	000719-32-4	719324	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000634-93-5	Nc(c(cc(c1)Cl)Cl)c1Cl	cl	0.00444	0.591951316
000635-22-3	O=N(=O)c(c(ccc1N)Cl)c1	cl	0.000412	0.054928816
000636-30-6	Nc(c(cc(c1Cl)Cl)Cl)c1	cl	0.00192	0.255978947
000719-32-4	O=C(c(c(c(c(c1Cl)C(=O)Cl)Cl)Cl)c1Cl)Cl	Cl	4.72E-06	6.29E-04

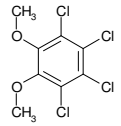
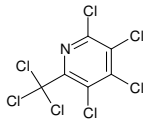
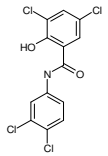
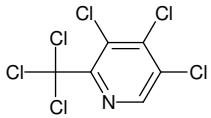
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000634-93-5	115.4280323	-4.499269073	3.01	4.114981685	102.4	2.010
000635-22-3	46.74031461	-6.642715581	2.12	5.368428192	7.695	0.886
000636-30-6	19.88437327	-4.499269073	3.01	4.114981685	90.47	1.957
000719-32-4	338.37	-4.40	3.46	7.86	92	1.962653405

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000634-93-5	P - triCl	neutral	N	Y	
000635-22-3	P - Cl, nitro	neutral	N	Y	
000636-30-6	P - triCl	amine	N	Y	
000719-32-4	tetrachloroterephthaloyl chloride. Use as chemical intermediate? Will hydrolyze rapidly to acid - No reports in 1998 and 2002. - no longer used - released from old products?	acid	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000634-93-5				N	0.5	0.5			
000635-22-3				N	0.5	0.5	0.5	0.5	
000636-30-6				N	0.5		0.5		
000719-32-4		tetrachlorodibenzoic acid	Y	N	10	10	10		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000634-93-5		Y	8.469	Fish 96-hour LC_{50} (mg/L)	moderate
000635-22-3		Y	21.714	Fish 96-hour LC_{50} (mg/L)	High-moderate
000636-30-6		Y	8.469	Fish 96-hour LC_{50} (mg/L)	moderate
000719-32-4		Y	9.47E+00	Fish 96-hour LC_{50} (mg/L)	Moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000634-93-5	634935	airbreather	Neutral Organics
000635-22-3	635223	airbreather	Esters
000636-30-6	636306	airbreather	Phenols
000719-32-4	719324		Esters

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000944-61-6	944616	
	001134-04-9	1134049	
	001154-59-2	1154592	
	001201-30-5	1201305	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000944-61-6	COc1c(Cl)c(Cl)c(Cl)c(Cl)c1OC	Cl	3.71E-04	4.95E-02
001134-04-9	n(c(c(c(c1Cl)Cl)Cl)C(Cl)(Cl)Cl)c1Cl	Cl	8.36E-05	1.11E-02
001154-59-2	O=C(Nc(ccc(c1Cl)Cl)c1)c(c(O)c(cc2Cl)Cl)c2	Cl	3.03E-10	4.04E-08
001201-30-5	n(c(c(c(c1Cl)Cl)Cl)C(Cl)(Cl)Cl)c1	Cl	0.000464	0.061861579

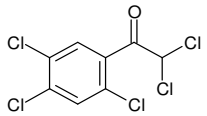
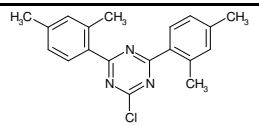
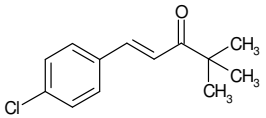
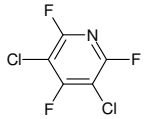
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000944-61-6	4.38	-3.63	4.22	7.85	1102	3.042181595
001134-04-9	3739.86	-4.58	5.29	9.87	2343	3.369772289
001154-59-2	3.60	-8.71	5.87	14.58	2652	3.42357352
001201-30-5	13098.01928	-5.24869169	4.64	6.494404301	747.3	2.873

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000944-61-6	tetrachloroveratrole. Chlorination byproduct.	neutral	Y	Y	
001134-04-9	Trichloromethyl group my hydrolyse	neutral	N	Y	
001154-59-2	3,3',4',5-Tetrachlorosalicylanilide. Used as a microbicide. May be analysable by LC-MS as anion or GCMS after derivatization.	phenol	N	N	Y
001201-30-5	Three Cl on benzyl C may chemically hydrolyze	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000944-61-6				Y					
001134-04-9				N	1				
001154-59-2				N					
001201-30-5		pyridinol?	Y	N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000944-61-6		Y	1.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
001134-04-9		Y	1.76E-01	Fish 96-hour LC_{50} (mg/L)	
001154-59-2		Y	0.076	Fish 96-hour LC_{50} (mg/L)	
001201-30-5		Y	0.114	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000944-61-6	944616		Esters + Esters (phosphate)
001134-04-9	1134049		Acrylamides
001154-59-2	1154592		Neutral Organics
001201-30-5	1201305	MPV	amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001203-86-7	1203867	
	001237-53-2	1237532	
		1577033	
5. Top 10 chlorinated	001737-93-5	1737935	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001203-86-7	O=C(c(c(cc(c1Cl)Cl)Cl)c1)C(Cl)Cl	cl	0.0000645	0.008599293
001237-53-2	Clc1nc(nc(n1)c2ccc(cc2C)C)c3ccc(cc3C)C	cl	3.43E-09	4.57296E-07
	CC(C)(C)C(=O)/C=C/c1ccc(Cl)cc1	Cl		
001737-93-5	Clc(c(F)nc1F)c(F)c1Cl	Cl	1.56E+00	2.08E+02

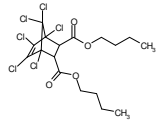
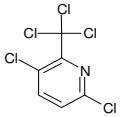
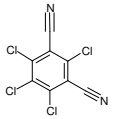
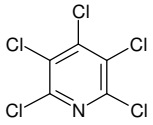
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
001203-86-7	274.9091686	-4.693965577	4.04	5.339678189	37.33	1.572
001237-53-2	7.421021293	-6.494809014	4.35	7.450521626	213	2.328
	1.09	-4.081445469	4.04	8.121	259.4	2.410
001737-93-5	172.54	-4.60	2.69	7.29	24	1.374931554

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001203-86-7	P - three Cl on ring	neutral	N	Y	
001237-53-2	P? - triazine ring, substituted benzenes	neutral	N	Y	
		neutral	N	Y	
001737-93-5	very persistent (five halogens on a pyridine ring - KOWWIN only 2.69 - use as chemical intermediate; may be occupational exposure measurements	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001203-86-7		benzoate	Y	N	10				
001237-53-2				N				0.5	
		Y	Y	N					No Reports
001737-93-5				N			0.5	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001203-86-7		Y	0.837	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
001237-53-2		Y	0.193	Fish 96-hour LC_{50} (mg/L)	Low-moderate
	>1M - 10M		1.30E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001737-93-5		Y	5.93E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
001203-86-7	1203867	airbreather	Neutral Organics
001237-53-2	1237532	airbreather	Neutral Organics
			Acid Chloride/Halide
001737-93-5	1737935		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
5. Top 10 chlorinated	001770-80-5	1770805	
	001817-13-6	1817136	
	001897-45-6	1897456	
	002176-62-7	2176627	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001770-80-5	CCCCOC(=O)C1C(C(=O)OCCCC)C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl	Cl	1.22E-07	1.63E-05
001817-13-6	n(c(c(cc1)Cl)C(Cl)(Cl)Cl)c1Cl	cl	0.00288	0.383968421
001897-45-6	N#Cc(c(c(c(c1C#N)Cl)Cl)Cl)c1Cl	cl	0.000000472	6.29282E-05
002176-62-7	n(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl	Cl	7.85E-04	1.05E-01

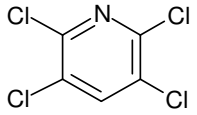
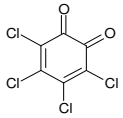
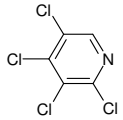
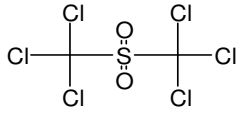
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
001770-80-5	320.20	-6.158	7.25	13.41	29340	4.46746011
001817-13-6	9221.306681	-3.316688769	4	3.92240138	238.4	2.377
001897-45-6	20770.32184	-5.206727188	3.66	5.4724398	44.51	1.648
002176-62-7	974.13	-0.59	4.03	4.62	104	2.018284308

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001770-80-5	Dibutyl chlorendate, flame retardant. May be amenable to GC-MS if esters are stable.	neutral	N	Y	
001817-13-6	P in air, triClmethyl should hydrolyze, Big production	neutral	N	Y	
001897-45-6	P in air, no production data - only DSL	neutral	N	Y	
002176-62-7	Like other chloropyridines, lLooks P - pesticide intermediate?	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001770-80-5		dicarboxylate	Y	N				0.5	0.5
001817-13-6		pyridinol?	Y	N	0.5	10	10	10	10
001897-45-6				N					
002176-62-7				N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001770-80-5		Y	0.006	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
001817-13-6		Y	0.146	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001897-45-6			2.136	Mysid Shrimp 96-hour LC_{50} (mg/L)	moderate
002176-62-7		Y	6.57E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
001770-80-5	1770805		Neutral Organics
001817-13-6	1817136	airbreather	Acid Chloride/Halide
001897-45-6	1897456	airbreather	Neutral Organics
002176-62-7	2176627		Vinyl/Allyl Ethers

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002402-79-1	2402791	
	002435-53-2	2435532	
	002808-86-8	2808868	
	003064-70-8	3064708	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002402-79-1	n(c(c(cc1Cl)Cl)Cl)c1Cl	Cl	6.06E-03	8.08E-01
002435-53-2	O=C(C(=C(C(=C1Cl)Cl)Cl)Cl)C1=O	Cl	0.000354	0.047196118
002808-86-8	n(c(c(c(c1Cl)Cl)Cl)Cl)c1	Cl	0.0173	2.306476974
003064-70-8	O=S(=O)(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl	Cl	0.00108	0.143988158

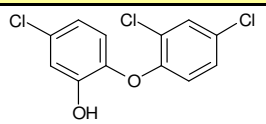
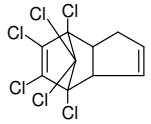
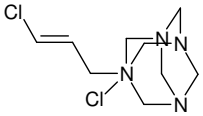
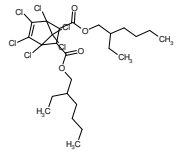
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
002402-79-1	685.20	-0.46	3.38	3.78	72	1.856426772
002435-53-2	1539.464968	-6.522283437	2.63	5.757996049	21.24	1.327
002808-86-8	8222.971748	-2.261465978	3.38	2.247178589	80.26	1.904
003064-70-8		-6.313023815	3.08	5.998736426	47.33	1.675

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002402-79-1	Like other chloropyridines, looks persistent, LOGKOW 3.38 not a big B	neutral	N	Y	
002435-53-2	P? - AO half-life high, Photolysis?	neutral	N	Y	
002808-86-8	Probably P - pesticide intermedia	neutral	N	Y	
003064-70-8	P - in air, not hydrogen abstraction, no production data - DSL	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002402-79-1				N	500	50	50	50	50
002435-53-2				N	0.5				
002808-86-8				N					0.5
003064-70-8				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002402-79-1		Y	1.04E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
002435-53-2		Y	15.358	Fish 96-hour LC_{50} (mg/L)	moderate
002808-86-8		Y	0.202	Fish 96-hour LC_{50} (mg/L)	
003064-70-8		Y	11.848	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
002402-79-1	2402791		Neutral Organics
002435-53-2	2435532	airbreather	Methacrylates
002808-86-8	2808868	MPV	Neutral Organics
003064-70-8	3064708	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	003380-34-5	3380345	
	003734-48-3	3734483	
	004080-31-3	4080313	
	004827-55-8	4827558	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
003380-34-5	O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl)c2	cl	0.00000465	0.000619949
003734-48-3	ClC1=C(Cl)C(Cl)(C2(Cl)Cl)C3CC=CC3C12Cl	Cl	2.07E-04	2.76E-02
004080-31-3	ClC=CCN(Cl)(CN(C1)C2)(CN1C3)CN32	Cl	4.19E-09	5.59E-07
004827-55-8	O=C(OCC(CCCC)CC)C(C(C(=C(C12Cl)Cl)Cl)(C1(Cl)Cl)Cl)C2C(=O)OCC(CCCC)CC	Cl	3.61E-10	4.81E-08

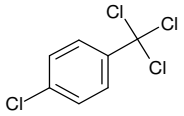
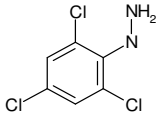
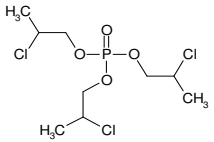
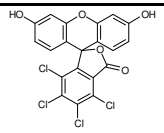
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
003380-34-5	7.965419774	-6.69047023	4.66	7.956182842	367.5	2.565
003734-48-3	0.04	-1.69	5.68	7.37	3082	3.488832634
004080-31-3	0.02	-6.14	-5.92	0.22	3	0.499961866
004827-55-8	320.20	-5.17	11.03	16.20	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
003380-34-5	P? three Cl, use? Big production; triclosan	phenol	N	N	Y
003734-48-3	Chlordene. Related to legacy OCP chlordane. One of several derivatives of hexachlorocyclopentadiene, no recent production	neutral	Y	Y	
004080-31-3	Interesting structure adamantane with N at all the bridge heads, quaternary Nitrogen?	neutral	N	Y	
004827-55-8	Di-2-Ethylhexyl Chlorendate, flame retardant. May be amenable to GC-MS if esters are stable.	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
003380-34-5				N	0.5	0.5	1	10	
003734-48-3				Y	50	10			
004080-31-3				N	10			0.5	
004827-55-8		dicarboxylate	Y	N	0.5	0.5	0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
003380-34-5			0.071	Fish 96-hour LC_{50} (mg/L)	Low-moderate
003734-48-3		Y	0.054	Fish 96-hour LC_{50} (mg/L)	High-moderate
004080-31-3		Y	2.57E+06	Fish 96-hour LC_{50} (mg/L)	
004827-55-8		Y	7.11E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
003380-34-5	3380345	airbreather	Acrylates
003734-48-3	3734483		Dinitrobenzenes
004080-31-3	4080313		Neutral Organics
004827-55-8	4827558		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	005216-25-1	5216251	
	005329-12-4	5329124	
	006145-73-9	6145739	
	006262-21-1	6262211	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
005216-25-1	c(ccc(c1)Cl)(c1)C(Cl)(Cl)Cl	Cl	0.0249	3.319726974
005329-12-4	N(N)c(c(cc(c1)Cl)Cl)c1Cl	Cl	0.00108	0.143988158
006145-73-9	O=P(OCC(C)Cl)(OCC(C)Cl)OCC(C)Cl	Cl	0.0000526	0.007012757
006262-21-1	O=C(OC(c(c(Oc1cc(O)cc2)cc(O)c3)c3)(c12)c4c(c(c(c5Cl)Cl)Cl)Cl)c45	Cl	1.08E-15	1.43988E-13

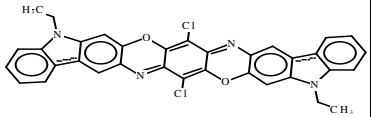
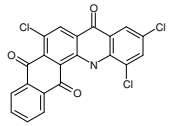
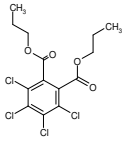
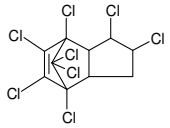
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
005216-25-1	510.7252974	-2.103013467	4.54	3.248726079	625.3	2.796
005329-12-4	115.4280323	-6.878025766	2.73	6.213738377	25.14	1.400
006145-73-9	5.451502575	-5.613324516	2.89	5.109037128	5.528	0.743
006262-21-1	0.640905677	-14.9588185	5.93	17.49453111	7330	3.865

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
005216-25-1	P - in air, hydrolysis of trichloromethyl, big production	neutral	N	Y	
005329-12-4	P? - triCl, photolysis of hydrazine? check analogs	amine	N	Y?	
006145-73-9	P? should be some data	neutral	Y	Y	
006262-21-1	P looking B possible. Use? Spiro intermediate	phenol	N	N	Y?

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
005216-25-1		carboxylate?	Y	N	100	100	50	50	
005329-12-4				N	0.5	0.5	0.5		
006145-73-9				N	10	10		0.5	
006262-21-1				N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
005216-25-1		Y	0.093	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
005329-12-4		Y	0.461	Fish 96-hour LC_{50} (mg/L)	Low-moderate
006145-73-9	-	Y	12.541	Mysid Shrimp 96-hour LC_{50} (mg/L)	moderate
006262-21-1			0.223	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
005216-25-1	5216251	airbreather	amides
005329-12-4	5329124	airbreather	Phenols
006145-73-9	6145739	airbreather	Esters
006262-21-1	6262211	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	006358-30-1	6358301	
	006373-31-5	6373315	
	006928-67-2	6928672	
	012789-03-6	12789036	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
006358-30-1	c1cc2N(CC)c3cc4OC5=C(Cl)C6=Nc7cc8c9ccccc9N(CC)c8cc7OC6=C(Cl)C5=Nc4cc3c2cc1	Cl	7.71E-18	1.03E-15
006373-31-5	c12Nc3c4C(=O)c5ccccc5C(=O)c4c(Cl)cc3C(=O)c1cc(Cl)cc2Cl	Cl	7.17E-13	9.56E-11
006928-67-2	O=C(OCCC)c(c(c(c(c1Cl)Cl)Cl)C(=O)OCCC)c1Cl	Cl	1.46E-06	1.95E-04
012789-03-6	ClC(C(Cl)C1)C(C1C2(Cl)C=3Cl)C(Cl)(C3Cl)C2(Cl)Cl	Cl	2.00E-05	2.67E-03

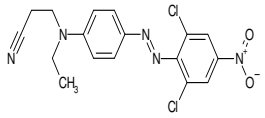
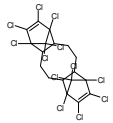
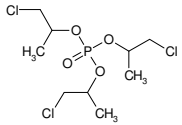
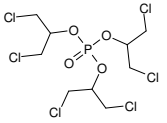
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
006358-30-1	0.04	-10.30	9.44	19.74	29	1.463
006373-31-5	6.01	-13.77	6.07	19.84	1361	3.134
006928-67-2	1.69	-5.07	6.21	11.28	11980	4.078
012789-03-6	2.11	-2.54	6.26	8.80	12290	4.090

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
006358-30-1	Pigment violet 23. Pigment and dye. Likely amenable to LC-MS	amine	N	N	
006373-31-5	Benzadone Red Violet 2. Pigment and dye. May be analyseable by GC-MS	neutral	N	Y	
006928-67-2	Likely to hydrolyse to diacid. May be analysable by GC-MS as the ester	neutral	N	Y	
012789-03-6	chlordane, OCP; legacy chemical banned in the 1980s	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
006358-30-1	Y			N	0.5	1	1	10	10
006373-31-5				N					
006928-67-2		tetrachlorophthalic acid	Y	N					
012789-03-6				Y					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
006358-30-1		N	6.08E-05	Fish 96-hour LC_{50} (mg/L)	
006373-31-5		Y	7.49E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
006928-67-2		Y	0.033	Mysid Shrimp 96-hour LC_{50} (mg/L)	Moderate
012789-03-6		Y	0.021	Fish 96-hour LC_{50} (mg/L)	High-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
006358-30-1	6358301		Esters
006373-31-5	6373315		Neutral Organics
006928-67-2	6928672		Acrylates
012789-03-6	12789036		Acrylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	013301-61-6	13301616	
5. Top 10 chlorinated	013560-89-9	13560899	
	013674-84-5	13674845	
	013674-87-8	13674878	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
013301-61-6	N(=O)(=O)c(cc(c(N=Nc(ccc(N(CCC(#N))CC)c1)c1)c2Cl)Cl)c2	Cl	1.40E-10	1.87E-08
013560-89-9	C(=C(C(C1(Cl)Cl)(C(C2CCC(C(C(=C(C34Cl)Cl)Cl)(C3(Cl)Cl)Cl)C4C5)C5)Cl)Cl)(C12Cl)Cl	Cl	7.06E-10	9.41E-08
013674-84-5	O=P(OC(CCl)C)(OC(CCl)C)OC(CCl)C	Cl	5.64E-05	7.52E-03
013674-87-8	O=P(OC(CCl)CCl)(OC(CCl)CCl)OC(CCl)CCl	Cl	2.86E-07	3.81E-05

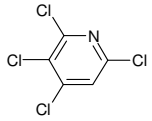
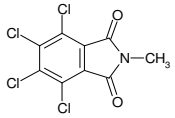
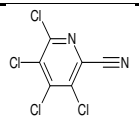
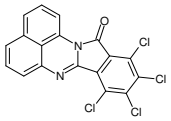
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
013301-61-6	0.00	-10.82	5.98	16.80	1	0.000
013560-89-9	160.10	-3.52	11.27	14.79	1	-0.301
013674-84-5	0.24	-5.61	2.89	8.50	3	0.514
013674-87-8	0.59	-6.97	3.65	10.62	21	1.330

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
013301-61-6	Pigment and dye. May be amenable to GC-MS analysis	neutral	N	Y	
013560-89-9	Dechlordane Plus ®. Has been measured in Great Lakes samples.	neutral	Y	Y	
013674-84-5	Phosphate based flame retardant and potential Penta BDE replacement. There are other chloroalkyl phosphate esters that may be of more concern - see 13674-87-8	neutral	Y	Y	
013674-87-8	Phosphate based flame retardant and potential Penta BDE replacement.	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
013301-61-6				N	0.5	0.5	0.5	10	0.5
013560-89-9				Y	10	10	10	10	10
013674-84-5				N	10	50	50	50	50
013674-87-8				N	10	10	50	50	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
013301-61-6		Y	8.88E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	High-moderate
013560-89-9		N	1.89E-06	Fish 96-hour LC_{50} (mg/L)	
013674-84-5		Y	1.27E+01	Fish 96-hour LC_{50} (mg/L)	Moderate
013674-87-8		Y	4.73E+00	Fish 96-hour LC_{50} (mg/L)	High-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
013301-61-6	13301616		Neutral Organics
013560-89-9	13560899		Neutral Organics
013674-84-5	13674845		Acrylates
013674-87-8	13674878		Thiols(mercaptans)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	014121-36-9	14121369	
	014737-80-5	14737805	
	017824-83-8	17824838	
	020749-68-2	20749682	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
014121-36-9	n(c(cc(c1Cl)Cl)Cl)c1Cl	Cl	0.0173	2.306476974
014737-80-5	O=C(N(C(=O)c1c(c(c(c2Cl)Cl)Cl)Cl)C)c12	cl	1.18E-08	1.5732E-06
017824-83-8	N#Cc(nc(c(c1Cl)Cl)Cl)c1Cl	Cl	1.89E-04	2.52E-02
020749-68-2	O=C(N(c(c(c(ccc1)cc2)c1N=3)c2)C3c4c(c(c(c5Cl)Cl)Cl)Cl)c45	Cl	1.7E-11	2.26648E-09

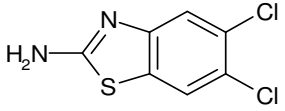
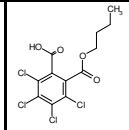
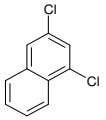
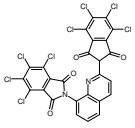
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
014121-36-9	3412.937756	-0.461200413	3.38	3.841	80.26	1.904
014737-80-5	8.233938025	-6.557982107	4.09	7.253694719	279.9	2.447
017824-83-8	3875.36	-4.27	2.93	7.20	36	1.556
020749-68-2	3.375316572	-9.081074738	5.18	10.86678735	1937	3.287

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
014121-36-9	P, not B. Degradation product/intermediate of pesticide	neutral	N	Y	
014737-80-5	P? No production - DSL, imide should hydrolysis, tetraCl	neutral	N	Y	
017824-83-8	Chloropyridine. Looks very P. Use - pesticide intermediate? Could be metabolite when pesticide is used e.g. pyridinol.	neutral	N	Y	
020749-68-2	P & B. Check use	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
014121-36-9				N		0.5	0.5	0.5	0.5
014737-80-5				N					
017824-83-8				N	10	10	10	10	10
020749-68-2				N		0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
014121-36-9		Y	0.202	Fish 96-hour LC_{50} (mg/L)	
014737-80-5			2.024	Fish 96-hour LC_{50} (mg/L)	
017824-83-8		Y	0.226	Fish 96-hour LC_{50} (mg/L)	Low-moderate
020749-68-2		Y	0.161	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
014121-36-9	14121369	MPV	Thiols(mercaptans)
014737-80-5	14737805	airbreather	Neutral Organics
017824-83-8	17824838		Neutral Organics
020749-68-2	20749682	MPV	Esters

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	024072-75-1	24072751	
	024261-19-6	24261196	
	028699-88-9	28699889	
	030125-47-4	30125474	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
024072-75-1	N=C(Nc(c1cc(c2Cl)Cl)c2)S1	cl	0.0000205	0.002733109
024261-19-6	O=C(OCCCC)c(c(c(c(c1Cl)Cl)Cl)C(=O)O)c1Cl	Cl	4.34E-08	5.78619E-06
028699-88-9	Clc1c2c(cc(c1)Cl)cccc2	Cl	1.41E-03	1.88E-01
030125-47-4	O=C2(c1(c(Cl)c(Cl)c(Cl)c(Cl)c1C(=O)N2c6(c5(nc(C4(C(=O)c3(c(Cl)c(Cl)c(Cl)c(Cl)c3C4(=O))))ccc5ccc6))))	Cl	1.76E-21	2.34647E-19

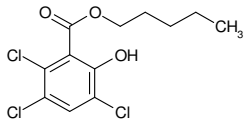
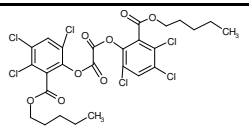
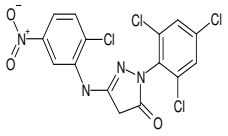
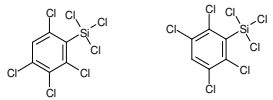
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
024072-75-1	23.85458896	-7.564444942	3.39	7.560157554	81.31	1.910
024261-19-6	25.19586555	-7.695723857	4.66	8.961436468	3.162	0.500
028699-88-9	2.41	-1.93	4.46	6.39	2252	3.353
030125-47-4	3.513375839	-17.65377095	10.18	24.43948356	3.162	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
024072-75-1	P? two Cl	neutral	N	Y	
024261-19-6	per Cl = P	acid	N	N	Y
028699-88-9	Dichloronaphthalene. Chloronaphthalenes have been monitored in Great Lakes samples	neutral	Y	Y	
030125-47-4	Looks very persistent. Too big for B. P metabolites?	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
024072-75-1				N		0.5	0.5	0.5	
024261-19-6	Y	dicarboxylate	Y	N		0.5			
028699-88-9				Y					
030125-47-4		tetrachlorophthalate	Y	N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
024072-75-1		Y	3.74	Mysid Shrimp 96-hour LC_{50} (mg/L)	
024261-19-6			5.24	Mysid Shrimp 96-hour LC_{50} (mg/L)	
028699-88-9		N	3.50E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
030125-47-4			7.80E-05	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
024072-75-1	24072751	airbreather	******> SMILES NOTATION PROBLEM: 68867629
024261-19-6	24261196	MPV	Neutral Organics
028699-88-9	28699889		Phenols
030125-47-4	30125474	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	030431-53-9	30431539	
	030431-54-0	30431540	
	030707-68-7	30707687	
	033434-63-8	33434638	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
030431-53-9	O=C(OCCCCC)c(c(c(cc1Cl)Cl)Cl)c1O	Cl	6.86E-07	9.15E-05
030431-54-0	O=C(Oc(c(cc(c1Cl)Cl)Cl)c1C(=O)OCCCCC)C(=O)Oc(c(cc(c2Cl)Cl)Cl)c2C(=O)OCCCCC	Cl	1.76E-14	2.34647E-12
030707-68-7	O=C(N(N=C1Nc(c(ccc2N(=O)=O)Cl)c2)c(c(cc(c3)Cl)Cl)c3Cl)C1	Cl	4.94E-12	6.59E-10
033434-63-8	Cl[Si](c1c(c(cc(c1Cl)Cl)Cl)Cl)(Cl)Cl	Cl	2.44E-04	3.25E-02

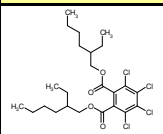
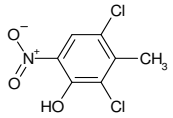
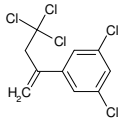
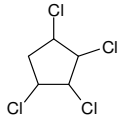
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
030431-53-9	1.74	-4.63	6.50	11.13	8057	3.906
030431-54-0	10.64866365	-9.038322758	9.32	14.96403537	3.162	0.500
030707-68-7	5.36	-13.73	5.26	18.99	2230	3.348
033434-63-8	130.04	-3.39	6.18	9.57	11480	4.060

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
030431-53-9	Likely to hydrolyse to chlorobenzoate. May be analysable by GC-MS if methylated	phenol	N	N	Y
030431-54-0	Not P but P metabolites	neutral	N	Y?	
030707-68-7	1-(2',4',6'-Trichlorophenyl)-3-(2'-chloro-5'-nitroanilino)-5-pyrazolone. Use is unknown. Looks amenable to GC-MS analysis	neutral	N	Y	
033434-63-8	Chemical reagent - will hydrolyse very rapidly in presence of water.	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
030431-53-9		2-hydroxy-3,5,6-trichlorobenzoate	Y	N	0.5	0.5	0.5	0.5	
030431-54-0		trichlorophenolate?	Y	N	0.5	0.5	0.5	0.5	
030707-68-7				N	0.5	0.5	0.5		
033434-63-8		Chlorophenol?	Y	N	0.5				0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
030431-53-9		N	0.015	Mysid Shrimp 96-hour LC_{50} (mg/L)	
030431-54-0			0.015	Mysid Shrimp 96-hour LC_{50} (mg/L)	
030707-68-7		Y	6.40E-02	Fish 96-hour LC_{50} (mg/L)	
033434-63-8		N	4.45E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
030431-53-9	30431539		Neutral Organics
030431-54-0	30431540	MPV	Dinitrobenzenes
030707-68-7	30707687		Neutral Organics
033434-63-8	33434638		Dinitrobenzenes

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	034832-88-7	34832887	
	039549-27-4	39549274	
	056984-96-4	56984964	
	059808-78-5	59808785	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
034832-88-7	O=C(OCC(CCCC)CC)c(c(c(c(c1Cl)Cl)Cl)C(=O)OCC(CCCC)CC)c1Cl	Cl	8.49E-10	1.13191E-07
039549-27-4	O=N(=O)c(c(O)c(c(c1Cl)C)Cl)c1	cl	0.0000198	0.002639783
056984-96-4	C=C(c1ccc(c(c1)Cl)C)CC(Cl)(Cl)Cl	Cl	0.000704	0.093858947
059808-78-5	ClC1C(C(CC1Cl)Cl)Cl	Cl	1.00E-01	1.33E+01

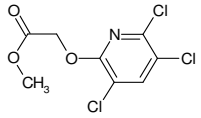
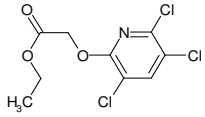
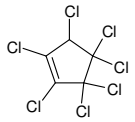
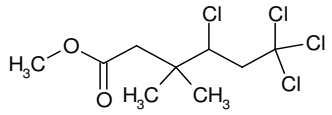
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
034832-88-7	5.882975747	-3.837120778	10.97	11.41283339	3.162	0.500
039549-27-4	369.7554054	-3.761204919	3.74	4.106917531	60.71	1.783
056984-96-4	2.413643246	-2.076816915	6.48	5.162529527	19510	4.290
059808-78-5	17.32	-1.20	3.41	4.61	84	1.923

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
034832-88-7	P metabolite, not B	neutral	N	Y	
039549-27-4	P - two Cl, one Nitro, pKa?	phenol	N	N	Y
056984-96-4	Might be P & B. Monomer? Olefin may be reactive	neutral	N	Y	
059808-78-5	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. P but no B. Use as intermediate?	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
034832-88-7		tetrachlorophthalate	Y	N				0.5	0.5
039549-27-4	Y			N	0.5				
056984-96-4		carboxylate?	Y	N		0.5			
059808-78-5				N	0.5	0.5	0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
034832-88-7		Y	6.87E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
039549-27-4		Y	1.748	Fish 96-hour LC_{50} (mg/L)	High-moderate
056984-96-4			0.00102	Mysid Shrimp 96-hour LC_{50} (mg/L)	
059808-78-5		Y	7.68E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
034832-88-7	34832887	MPV	Neutral Organics
039549-27-4	39549274	airbreather	Phenols (dinitro)
056984-96-4	56984964	MPV	Neutral Organics
059808-78-5	59808785		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	060825-26-5	60825265	
	060825-27-6	60825276	
5. Top 10 chlorinated	062111-47-1	62111471	
	064667-33-0	64667330	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
060825-26-5	O=C(OC)COc(nc(c(c1)Cl)Cl)c1Cl	cl	0.00012	0.015998684
060825-27-6	Clc1nc(c(cc1Cl)Cl)OCC(=O)OCC	cl	0.0000484	0.006452803
062111-47-1	ClC1(C(C(Cl)C(=C1Cl)Cl)(Cl)Cl)Cl	Cl	5.07E-03	6.76E-01
064667-33-0	O=C(OC)CC(C(Cl)CC(Cl)(Cl)Cl)(C)C	cl	0.00484	0.645280263

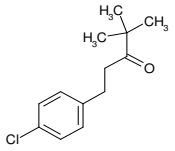
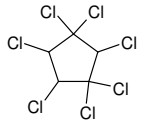
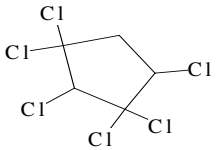
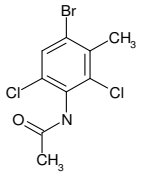
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
060825-26-5	63.23057132	-4.171086832	2.81	3.586799443	29.31	1.467
060825-27-6	36.94765552	-4.050114282	3.31	3.965826894	70.02	1.845
062111-47-1	2.66	-1.99	4.44	6.43	521	2.717
064667-33-0	62.71281463	-3.218309061	4.74	4.564021672	898.3	2.953

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
060825-26-5	P? ester will hydrolyze - 2,4,5-T analog	neutral	N	Y	
060825-27-6	Ethyl ester hydrolyzes. 2,4,5-T analog	neutral	N	Y	
062111-47-1	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. Use - olefin - polymer monomer?	neutral	N	Y	
064667-33-0	P for the acid, need estimates for acid, pKa	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
060825-26-5		pyridinol?	Y	N	10				
060825-27-6		pyridinol?	Y	N		10			10
062111-47-1				N			10	10	10
064667-33-0				N	10	10	10	10	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
060825-26-5		Y	0.252	Fish 96-hour LC_{50} (mg/L)	
060825-27-6			0.266	Fish 96-hour LC_{50} (mg/L)	
062111-47-1		Y	1.61E-01	Fish 96-hour LC_{50} (mg/L)	Low-moderate
064667-33-0		Y	0.369	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
060825-26-5	60825265	airbreather	Anilines (amino-meta)
060825-27-6	60825276	airbreather	Vinyl/Allyl Ketones
062111-47-1	62111471		Neutral Organics
064667-33-0	64667330	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	066346-01-8	66346018	
5. Top 10 chlorinated	068258-90-2	68258902	
	068258-91-3	68258913	
	068399-95-1	68399951	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
066346-01-8	O=C(C(C)(C)C)CCc1ccc(cc1)Cl	cl	0.00126	0.167986184
068258-90-2	ClC1(C(C(C(C1Cl)Cl)(Cl)Cl)Cl)Cl	Cl	2.54E-03	3.39E-01
068258-91-3	ClC1C(C(C(C1)(Cl)Cl)Cl)(Cl)Cl	Cl	2.04E-02	2.72E+00
068399-95-1	O=C(Nc(c(cc(c1C)Br)Cl)c1Cl)C	Cl	0.000000876	0.00011679

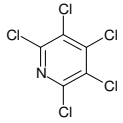
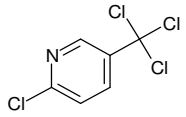
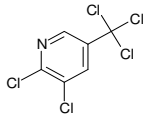
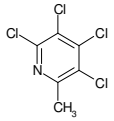
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
066346-01-8	16.52744785	-3.424311146	3.97	4.000023757	227.7	2.357
068258-90-2	93.49	-2.56	4.03	6.59	253	2.402
068258-91-3	46.84	-2.10	3.85	5.95	183	2.263
068399-95-1	204.5554477	-7.215384508	2.7	6.521097119	24.02	1.381

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
066346-01-8	May not be P - check use, very large production	neutral	N	Y	
068258-90-2	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. Use?	neutral	N	Y	
068258-91-3	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. Use?	neutral	N	Y	
068399-95-1	P (trihaloaniline), not B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
066346-01-8				N		10	10	10	10
068258-90-2				N			50	500	50
068258-91-3				N			50	50	10
068399-95-1				N					0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
066346-01-8			0.782	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068258-90-2		Y	1.93E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
068258-91-3		Y	2.88E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
068399-95-1			10.647	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
066346-01-8	66346018	airbreather	Neutral Organics
068258-90-2	68258902		Vinyl/Allyl Ketones
068258-91-3	68258913		Neutral Organics
068399-95-1	68399951	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
5. Top 10 chlorinated	068412-40-8	68412408	
	069045-78-9	69045789	
	069045-83-6	69045836	
	070024-85-0	70024850	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068412-40-8	n1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	Cl	7.85E-04	1.05E-01
069045-78-9	ClC(c1cnc(cc1)Cl)(Cl)Cl	cl	0.0198	2.639782895
069045-83-6	ClC(c1cnc(c(c1)Cl)Cl)(Cl)Cl	cl	0.00288	0.383968421
070024-85-0	n1c(Cl)c(Cl)c(Cl)c(Cl)c1C	Cl	5.25E-03	7.00E-01

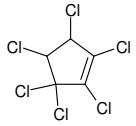
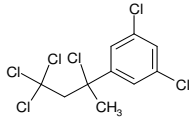
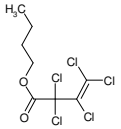
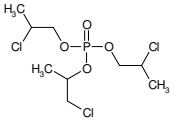
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068412-40-8	974.13	-0.59	4.03	4.62	104	2.018
069045-78-9	2691.561942	-3.187173652	3.35	3.142886263	76.03	1.881
069045-83-6	12547.46715	-3.316688769	4	3.92240138	238.4	2.377
070024-85-0	60.51	-2.22	3.93	6.15	212	2.326

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068412-40-8	Like other chloropyridines, looks persistent. Probably persistent. Uses - pesticide intermediate?	neutral	N	Y	
069045-78-9	P in air, CCl3 will chemically hydrolyze	neutral	N	Y	
069045-83-6	P in air, CCl3 will chemically hydrolyze	neutral	N	Y	
070024-85-0	Like other chloropyridines, looks persistent. Probably persistent. Uses - pesticide intermediate?	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068412-40-8				N	10	10	10	10	10
069045-78-9				N					
069045-83-6				N					
070024-85-0				N	1	10	10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068412-40-8		Y	1.56E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
069045-78-9		Y	0.185	Mysid Shrimp 96-hour LC_{50} (mg/L)	
069045-83-6			0.146	Mysid Shrimp 96-hour LC_{50} (mg/L)	
070024-85-0		Y	1.91E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
068412-40-8	68412408		Peroxy Acids
069045-78-9	69045789	airbreather	Esters + Esters (phosphate)
069045-83-6	69045836	airbreather	Neutral Organics
070024-85-0	70024850		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	072030-26-3	72030263	
	073588-42-8	73588428	
	075147-20-5	75147205	
	076649-15-5	76649155	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
072030-26-3	ClC1=C(Cl)C(C(C1(Cl)Cl)Cl)Cl	Cl	1.04E-02	1.39E+00
073588-42-8	Clc1cc(cc(c1)Cl)C(CC(Cl)(Cl)Cl)(C)Cl	Cl	1.48E-04	1.97E-02
075147-20-5	ClC(C(=C(Cl)Cl)Cl)(C(=O)OCCCC)Cl	Cl	1.69E-03	2.25E-01
076649-15-5	O=P(OC(CCl)C)(OCC(C)Cl)OCC(C)Cl	Cl	3.57E-05	4.76E-03

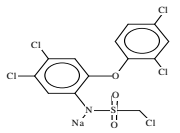
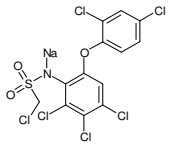
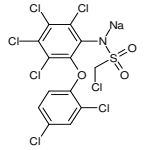
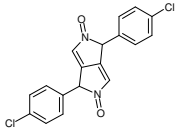
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
072030-26-3	3.31	-1.54	4.22	5.76	352	2.547
073588-42-8	4.60	-3.32	6.80	10.12	34420	4.537
075147-20-5	2.29	-2.99	5.14	8.13	1797	3.255
076649-15-5	0.00	-5.61	2.89	8.50	1	-0.129

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
072030-26-3	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. Use?	neutral	N	Y	
073588-42-8	Current use unknown. Comes from DSL. Looks analysable by GC-MS	neutral	N	Y	
075147-20-5	Current use unknown. Comes from DSL. Looks analysable by GC-MS	neutral	N	Y	
076649-15-5	Phosphate based flame retardant and potential Penta BDE replacement. There are other chloroalkyl phosphate esters that may be of more concern - see 13674-87-8	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
072030-26-3				N	50	50			
073588-42-8				N		1			
075147-20-5				N	0.5	1			
076649-15-5				N		0.5	0.5	10	1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
072030-26-3		Y	1.99E-01	Fish 96-hour LC_{50} (mg/L)	Low-moderate
073588-42-8		Y	0.037	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
075147-20-5		Y	0.147	Fish 96-hour LC_{50} (mg/L)	
076649-15-5		Y	8.90E+00	Fish 96-hour LC_{50} (mg/L)	Moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
072030-26-3	72030263		Phosphate acid
073588-42-8	73588428		Neutral Organics
075147-20-5	75147205		Neutral Organics
076649-15-5	76649155		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	083721-46-4	83721464	
	083721-47-5	83721475	
	083721-48-6	83721486	
	084632-65-5	84632655	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
083721-46-4	c1cc(Cl)cc(Cl)c1Oc2cc(Cl)c(Cl)cc2N([Na])S(=O)(=O)CCl	Cl	8.93E-18	1.19E-15
083721-47-5	ClCS(=O)(=O)N([Na])c2c(cc(c(c2Cl)Cl)Cl)Oc1c(cc(cc1)Cl)Cl	Cl	2.15E-18	2.87E-16
083721-48-6	c1cc(Cl)cc(Cl)c1Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2N([Na])S(=O)(=O)CCl	Cl	5.16E-19	6.88E-17
084632-65-5	Clc1ccc(cc1)C3=C2C(=O)NC(=C2C(=O)N3)c4ccc(cc4)Cl	Cl	2.36E-13	3.15E-11

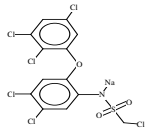
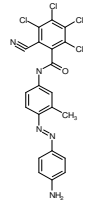
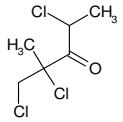
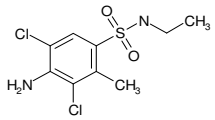
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
083721-46-4	2.12	-6.00	4.56	10.56	3792	3.579
083721-47-5	3.07	-6.13	5.20	11.33	11890	4.075
083721-48-6	3.04	-6.26	5.85	12.11	37270	4.571
084632-65-5	0.01	-12.93	2.20	15.13	10	0.993

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
083721-46-4	Use unknown. Pigment or dye? May degrade to aniline. No likely amenable to GC-MS due to N+ group. Possible LC-MS candidate (+ ion)	neutral	N	N	
083721-47-5	Use unknown. Pigment or dye? May degrade to aniline. No likely amenable to GC-MS due to N+ group. Possible LC-MS candidate (+ ion)	neutral	N	N	
083721-48-6	Use unknown. Pigment or dye? May degrade to aniline. No likely amenable to GC-MS due to N+ group. Possible LC-MS candidate (+ ion)	neutral	N	N	
084632-65-5	Pigment Red 25Colorant for food contact plastic. Possibly persistent. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
083721-46-4	Y	aniline of tetrachlorodiphenyl ether	Y	N					
083721-47-5	Y	aniline of pentachlorodiphenyl ether	Y	N					
083721-48-6	Y	aniline of hexachlorodiphenyl ether	Y	N					
084632-65-5				N		0.5	1	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
083721-46-4		Y	6.20E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
083721-47-5		Y	1.10E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
083721-48-6		Y	1.73E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
084632-65-5		Y	25.434	Fish, 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
083721-46-4	83721464		Neutral Organics
083721-47-5	83721475		Neutral Organics
083721-48-6	83721486		Neutral Organics
084632-65-5	84632655		Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	094248-26-7	94248267	
	106276-78-2	106276782	
	145556-04-3	145556043	
	151574-12-8	151574128	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
094248-26-7	ClCS(=O)(=O)N([Na])c1cc(Cl)c(Cl)cc1Oc2c(Cl)c(Cl)cc(Cl)c2	Cl	2.15E-18	2.87E-16
106276-78-2	N#Cc1c(Cl)c(Cl)c(Cl)c(Cl)c1C(=O)Nc2cc(C)c(cc2)N=Nc3ccc(cc3)N	Cl	1.28E-15	1.70653E-13
145556-04-3	O=C(C(Cl)(CCl)C)C(Cl)C	Cl	1.30E-01	1.73E+01
151574-12-8	O=S(=O)(c1c(c(c(c(c1)Cl)N)Cl)C)NCC	Cl	0.000000217	2.8931E-05

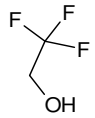
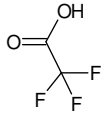
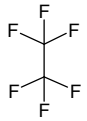
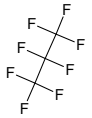
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
094248-26-7	2.37	-6.13	5.20	11.33	11890	4.075
106276-78-2	2.306613784	-15.80993157	6.57	18.98564418	10	1.000
145556-04-3	6.78	-3.68	1.82	5.50	5	0.698
151574-12-8	13.64989281	-7.966966849	2.25	6.822679461	10.71	1.030

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
094248-26-7	Use unknown. Pigment or dye? May degrade to aniline. No likely amenable to GC-MS due to N+ group. Possible LC-MS candidate (+ ion)	neutral	N	N	
106276-78-2	P metabolite tetra Cl, nitrile	amine	N	Y?	
145556-04-3	This looks very persistent - B is probably not high. Probably amenable to GC analysis	neutral	N	Y	
151574-12-8	P? two Cls. sulfonamide will degrade	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
094248-26-7	Y	aniline of pentachlorodiphenyl ether	Y	N					
106276-78-2		carboxylate	Y	N					0.5
145556-04-3				N			10	10	50
151574-12-8				N			0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
094248-26-7		Y	1.10E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
106276-78-2			0.051	Fish, 96-hour LC_{50} (mg/L)	
145556-04-3		Y	0.11	Fish, 96-hour LC_{50} (mg/L)	High-moderate
151574-12-8		Y	30.463	Fish, 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
094248-26-7	94248267		Neutral Organics
106276-78-2	106276782	MPV	Neutral Organics
145556-04-3	145556043		Neutral Organics
151574-12-8	151574128	airbreather	Acid Chloride/Halide

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000075-89-8	75898	
	000076-05-1	76051	
	000076-16-4	76164	
	000076-19-7	76197	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000075-89-8	FC(F)(F)CO	F	7.50E+01	1.00E+04
000076-05-1	O=C(O)C(F)(F)F	F	1.16E+02	1.55E+04
000076-16-4	FC(F)(F)C(F)(F)F	F	1.51E+04	2.01E+06
000076-19-7	FC(F)(F)C(F)(F)C(F)(F)F	F	5.34E+03	7.12E+05

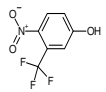
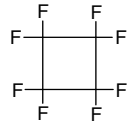
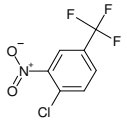
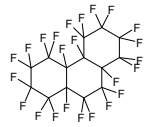
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000075-89-8	28.74	-2.94	0.27	3.21	3	0.500
000076-05-1	20.57	-3.75	0.50	4.25	3	0.500
000076-16-4		2.99	2.15	-0.84	7	0.840
000076-19-7		3.72	3.12	-0.60	50	1.703

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000075-89-8	P but not B. TFA degradation product; very volatile but probably amenable to GC analysis	neutral	N	Y	
000076-05-1	Trifluoro acetic acid. Widely measured.	acid	N	N	Y
000076-16-4	solvent? - release to environ.? - very persistent; GW too; very volatile but probably amenable to GC analysis	neutral	Y	Y	
000076-19-7	very volatile but probably amenable to GC analysis	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000075-89-8	Y	TFA	Y	N	1	1	10	10	10
000076-05-1				N	0.5	0.5	0.5	10	10
000076-16-4				N	0.5	0.5	0.5	10	10
000076-19-7				N	0.01		0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000075-89-8		Y	2542.99	Fish 96-hour LC_{50} (mg/L)	
000076-05-1		N	8683.693	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000076-16-4		N	69.377	Fish 96-hour LC_{50} (mg/L)	Low
000076-19-7		N	1.60E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000075-89-8	75898		Neutral Organics
000076-05-1	76051		amine
000076-16-4	76164		Benzyl Halides
000076-19-7	76197		Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000088-30-2	88302	
	000115-25-3	115253	
Top 10 fluorinated	000121-17-5	121175	
Top 10 fluorinated	000306-91-2	306912	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000088-30-2	Oc(ccc1N(=O)(=O))cc1C(F)(F)F	F	0.00146	0.194650658
000115-25-3	FC(F)(C(F)(F)C1(F)F)C1(F)F	F	2.16E+03	2.88E+05
000121-17-5	O=N(=O)c(c(ccc1C(F)(F)F)Cl)c1	F	0.118	15.73203947
000306-91-2	FC2(F)(C1(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C1(F)C3(F)(C(F)(C2(F)F)C(F)(F)C(F)(F)C(F)(F)C3(F)F)))	F	0.321	42.79648026

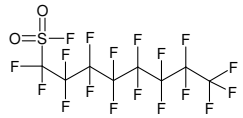
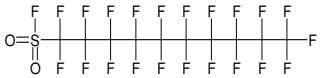
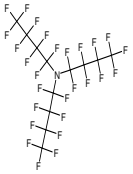
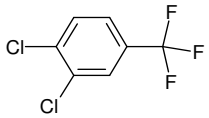
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000088-30-2	166.6328136	-6.105269547	2.87	5.580982159	32.42	1.511
000115-25-3		3.48	2.29	-1.19	12	1.066
000121-17-5	3724.915525	-2.251850209	3.42	2.27756282	85.51	1.932
000306-91-2		8.781690939	9.58	-2.595978328	18.88	1.276

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000088-30-2		phenol	N	N	Y
000115-25-3	solvent, GW, persistent. Very volatile but probably amenable to GC analysis	neutral	Y	Y	
000121-17-5	Probably very P but not B	neutral	N	Y	
000306-91-2	Perfluorinate = P. Unknown B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000088-30-2				N					
000115-25-3				N			0.5	10	10
000121-17-5				N	0.5	0.5			0.5
000306-91-2				N	0.5	0.5		0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000088-30-2		Y	7.107	Fish, 96-hour LC_{50} (mg/L)	Low-moderate
000115-25-3		N	1.86E+01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000121-17-5		Y	3.562	Mysid Shrimp 96-hour LC_{50} (mg/L)	High-moderate
000306-91-2		N	4.61E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000088-30-2	88302	airbreather	Neutral Organics
000115-25-3	115253		Neutral Organics
000121-17-5	121175	MPV	Neutral Organics
000306-91-2	306912	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000307-35-7	307357	
	000307-51-7	307517	
	000311-89-7	311897	
Top 10 fluorinated	000328-84-7	328847	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000307-35-7	O=S(=O)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	5.75E+00	7.67E+02
000307-51-7	O=S(=O)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	4.37E+00	5.83E+02
000311-89-7	FC(F)(N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F	F	1.06E+00	1.41E+02
000328-84-7	FC(F)(F)c(ccc(c1Cl)Cl)c1	F	1.32E+00	1.76E+02

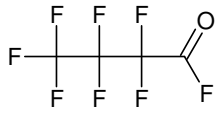
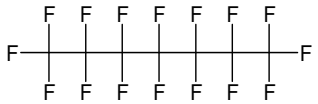
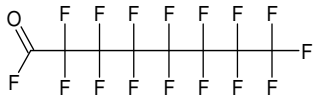
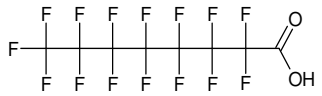
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000307-35-7		3.44	9.62	6.18	17	1.225
000307-51-7		3.89	11.55	7.66	3	0.500
000311-89-7		6.35	9.98	3.63	5	0.727
000328-84-7	132.87	0.02	4.24	4.22	370	2.569

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000307-35-7	Intermediate for production of perfluoro sulfonates. Now phased out by major manufacturer	acid	N	N	
000307-51-7	Intermediate for production of perfluoro sulfonates. Now phased out by major manufacturer	acid	N	N	
000311-89-7	Perfluorotributylamine. No reports on TSCA inventory since 1994; Persistent; probably amenable to GC-MS analysis	neutral	N	Y	
000328-84-7	3,4-Dichlorobenzotrifluoride. Looks very P, pesticide/drug intermediate?	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000307-35-7		PFOS	Y	N	10	10	10	10	0.5
000307-51-7		PFDS	Y	N		0.5	0.5		
000311-89-7				N	10	10			
000328-84-7				N	10	10	10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000307-35-7		N	0.006	Fish 96-hour LC_{50} (mg/L)	
000307-51-7		N	0.000838	Fish 96-hour LC_{50} (mg/L)	
000311-89-7		Y	0.000766	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000328-84-7		Y	7.30E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000307-35-7	307357		Neutral Organics
000307-51-7	307517		Phenols
000311-89-7	311897		anilines
000328-84-7	328847		Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000335-42-2	335422	
	000335-57-9	335579	
	000335-66-0	335660	
	000335-67-1	335671	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000335-42-2	O=C(F)C(F)(F)C(F)(F)C(F)(F)F	F	5.95E+02	7.93E+04
000335-57-9	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	8.74E+01	1.17E+04
000335-66-0	O=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.52E+01	2.03E+03
000335-67-1	O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.51E-01	2.01E+01

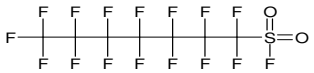
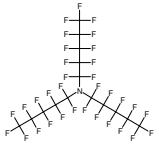
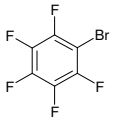
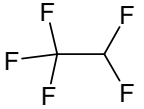
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000335-42-2		0.14	1.56	1.42	3	0.503
000335-57-9		5.60	6.99	1.39	47730	4.679
000335-66-0		3.02	5.43	2.41	3011	3.479
000335-67-1	20.57	-0.43	6.30	6.73	56	1.750

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000335-42-2	Perfluorobutanoic acid reactive intermediate/starting material	acid	N	N	
000335-57-9	very volatile but probably amenable to GC analysis; very volatile but probably amenable to GC analysis	neutral	Y	Y	
000335-66-0	Will degrade to PFHpA	acid	N	N	
000335-67-1	PFHpA	acid	Y	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000335-42-2		perfluoropropanoic acid	Y	N	0.5		0.5	10	10
000335-57-9				N	0.5	0.5	0.5		
000335-66-0		perfluoroheptanoic acid	Y	N	0.5	0.5	0.5	0.5	
000335-67-1	Y			Y	0.5		0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000335-42-2		Y	8.77E+01	Fish 96-hour LC_{50} (mg/L)	Moderate
000335-57-9		N	4.80E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000335-66-0		N	0.554	Fish 96-hour LC_{50} (mg/L)	
000335-67-1		Y	4.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000335-42-2	335422		Neutral Organics
000335-57-9	335579		Neutral Organics
000335-66-0	335660		Dinitrobenzenes
000335-67-1	335671		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000335-71-7	335717	
	000338-84-1	338841	
Top 10 fluorinated	000344-04-7	344047	
	000354-33-6	354336	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000335-71-7	O=S(=O)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	8.01E+00	1.07E+03
000338-84-1	FC(F)(N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.01E-02	2.68E+00
000344-04-7	Fc(c(c(F)c(F)c1F)Br)c1F	f	7.29	971.9200658
000354-33-6	FC(F)C(F)(F)F	F	7.12E+03	9.49E+05

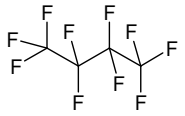
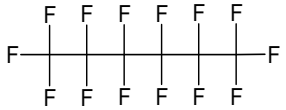
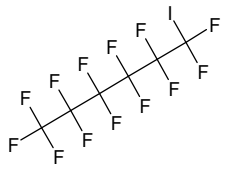
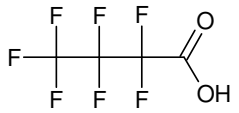
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000335-71-7		1.72	8.65	6.93	353	2.548
000338-84-1		7.51	12.88	5.37	3	0.500
000344-04-7	1025.735888	-0.721117823	3.88	1.206830435	195.6	2.291
000354-33-6	8767.20	2.10	1.55	-0.55	3	0.491

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000335-71-7	Will degrade to PFHpS	acid	N	N	
000338-84-1	see 311897; Persistent; probably amenable to GC-MS analysis	neutral	N	Y	
000344-04-7	Definitely P - not very B	neutral	N	Y	
000354-33-6	Pentafluoroethane. GWP concern but not PBT; very volatile. Amenable to GC analysis suitably modified for gases	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000335-71-7		PFHpS	Y	N	0.5	0.5	0.5	0.5	
000338-84-1				N	1	0.5			
000344-04-7				N				0.5	
000354-33-6				N			0.5	50	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000335-71-7		N	0.024	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000338-84-1		Y	2.87E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000344-04-7		Y	1.086	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate
000354-33-6		N	231.516	Fish 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000335-71-7	335717		Neutral Organics
000338-84-1	338841		amine
000344-04-7	344047	MPV	amine
000354-33-6	354336		amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000355-25-9	355259	
	000355-42-0	355420	
	355-43-1	355431	
	000375-22-4	375224	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000355-25-9	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.89E+03	2.52E+05
000355-42-0	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.39E+02	3.19E+04
355-43-1	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I	F		
000375-22-4	O=C(O)C(F)(F)C(F)(F)C(F)(F)F	F	1.50E+01	2.00E+03

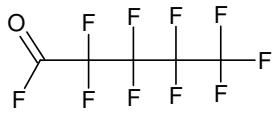
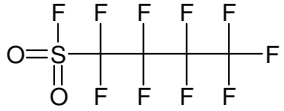
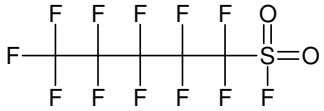
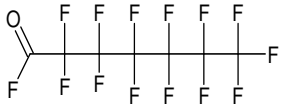
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000355-25-9		3.44	4.09	0.65	280	2.447
000355-42-0		4.88	6.02	1.14	8609	3.935
355-43-1	>100	2.635955056	6.84		36690	4.560
000375-22-4	20.57	-3.31	2.43	5.74	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000355-25-9	Perfluorobutane. Fully halogenated GWP and ODP ; atmospheric measurements. Amenable to GC analysis suitably modified for gases	neutral	Y	Y	
000355-42-0	gas GWP concern but not PBT; very volatile. Amenable to GC analysis suitably modified for gases	neutral	Y	Y	
355-43-1		neutral	N	Y	
000375-22-4	Perfluorobutanoic acid	acid	Y	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000355-25-9				N				0.5	0.5
000355-42-0				N	0.5	0.5		0.5	
355-43-1		Y	Y	N					No Reports
000375-22-4	Y			N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000355-25-9		N	1.24E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000355-42-0		N	6.82E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
355-43-1	>1M - 10M		8.50E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
000375-22-4		Y	1.33E+02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000355-25-9	355259		Neutral Organics
000355-42-0	355420		Benzyl Halides
355-43-1	355431		Benzyl Halides
000375-22-4	375224		Halo ketones

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000375-62-2	375622	
	000375-72-4	375724	
	000375-81-5	375815	
	000375-84-8	375848	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000375-62-2	O=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.41E+02	3.21E+04
000375-72-4	O=S(=O)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.68E+02	2.24E+04
000375-81-5	O=S(=O)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.20E+01	1.60E+03
000375-84-8	O=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	3.83E+01	5.11E+03

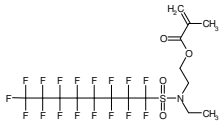
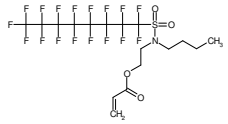
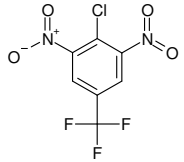
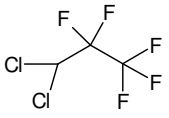
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000375-62-2		0.86	2.53	1.67	18	1.247
000375-72-4		-0.44	5.75	6.19	5364	3.729
000375-81-5		0.28	6.72	6.44	29740	4.473
000375-84-8		2.30	4.46	2.16	543	2.735

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000375-62-2	Will degrade to PFBA	acid	N	N	
000375-72-4	Intermediate for production of perfluorobutyl sulfonates; replacement chemistry for PFOS	acid	N	N	
000375-81-5	Will degrade to PFPnS	acid	N	N	
000375-84-8	Will degrade to PFHxS	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000375-62-2		PFBA	Y	N		0.5			
000375-72-4		PFBS	Y	N	0.5	0.5	0.5	0.5	0.5
000375-81-5		PFPnS	Y	N	0.5	0.5	0.5	0.5	
000375-84-8		PFHxS	Y	N		0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000375-62-2		N	2.75E+01	Fish 96-hour LC_{50} (mg/L)	
000375-72-4		N	0.279	Fish 96-hour LC_{50} (mg/L)	
000375-81-5		N	0.11	Fish 96-hour LC_{50} (mg/L)	
000375-84-8		N	2.48E+00	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000375-62-2	375622		Triazines
000375-72-4	375724		
000375-81-5	375815		Neutral Organics
000375-84-8	375848		Esters + Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000376-14-7	376147	
	000383-07-3	383073	
Top 10 fluorinated	000393-75-9	393759	
	000422-56-0	422560	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000376-14-7	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CC)C(=C)C	F	4.87E-05	6.49E-03
000383-07-3	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CCCC)C=C	F	1.87E-05	2.49E-03
000393-75-9	N(=O)(=O)c1c(Cl)c(N(=O)(=O))cc(C(F)(F)F)c1	F	3.81E-04	5.08E-02
000422-56-0	FC(C(F)(F)F)(C(Cl)Cl)F	F	2.80E+02	3.73E+04

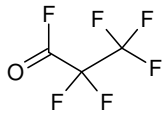
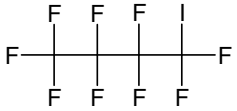
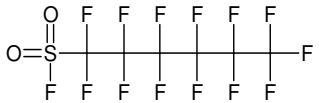
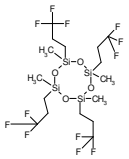
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000376-14-7	0.21	-0.90	9.69	10.59	14	1.131
000383-07-3	0.29	-0.85	10.12	10.97	3	0.535
000393-75-9	16206.04	-4.66	3.24	7.90	17	1.225
000422-56-0	2122.22	0.31	3.14	2.83	52	1.718

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000376-14-7	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. PFOS as degradation product	neutral	Y	N	
000383-07-3	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. PFOS as degradation product	neutral	Y	N	
000393-75-9	1-Chloro-2,6-Dinitro-4-(Trifluoromethyl) Benzene. Predicted to be very P, no recent Production	neutral	N	Y	
000422-56-0	1,1-Dichloro-2,2,3,3,3-pentafluoropropane. GWP concern but not PBT; very volatile but probably amenable to GC analysis	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000376-14-7	Y	PFOS	Y	N	0.5	0.5	0.5	0.5	0.5
000383-07-3	Y	PFOS	Y	N	0.5	0.5	0.5	0.5	0.5
000393-75-9				N	1	10	10		
000422-56-0				N				0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000376-14-7		N	0.000652	Fish 96-hour LC_{50} (mg/L)	
000383-07-3		N	0.1	Fish 96-hour LC_{50} (mg/L)	
000393-75-9		Y	1.99E+00	Fish 96-hour LC_{50} (mg/L)	Moderate
000422-56-0		Y	1.63E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000376-14-7	376147		Benzyl Halides
000383-07-3	383073		Neutral Organics
000393-75-9	393759		Neutral Organics
000422-56-0	422560		Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
		422617	
	000423-39-2	423392	
	000423-50-7	423507	
	000429-67-4	429674	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
	O=C(F)C(F)(F)C(F)(F)F	F		
000423-39-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)I	F	1.61E+02	2.15E+04
000423-50-7	O=S(=O)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	9.80E+00	1.31E+03
000429-67-4	[Si](O[Si](O[Si]1(C)CCC(F)(F)F)(C)CCC(F)(F)F)(O[Si](O1)(C)CCC(F)(F)F)(C)CCC(F)(F)F	F	7.49E-03	9.99E-01

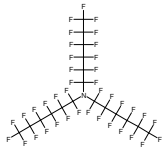
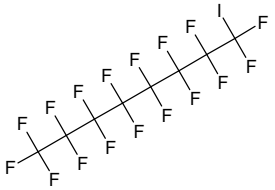
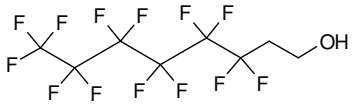
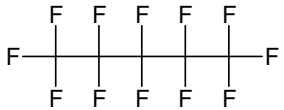
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
	>100	2.635955056	0.60		3.162	0.500
000423-39-2	a	2.31	4.90	2.59	1193	3.077
000423-50-7	a	1.00	7.68	6.68	7444	3.872
000429-67-4	1.79	4.12	10.68	6.56	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
		neutral	N	Y	
000423-39-2	Perfluorobutyl iodide. Very volatile but probably amenable to GC analysis	neutral	Y	Y	
000423-50-7	PFOS related product. Reactive starting material	acid	N	N	
000429-67-4	Fluorinated cyclic siloxane. May be analysable with other cyclic siloxanes by GC-MS. Highly volatile and persistent	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
				N					No Reports
000423-39-2				N			0.5	0.5	0.5
000423-50-7		PFHxS	Y	N	0.5	0.5	0.5	1	
000429-67-4				N		0.5	0.5	1	1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
	>500K - 1M		49.76	Fish 96-hour LC_{50} (mg/L)	moderate
000423-39-2		N	1.80E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
000423-50-7		N	0.043	Fish 96-hour LC_{50} (mg/L)	
000429-67-4		N	1.89E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
	422617		Halopyridines
000423-39-2	423392		Neutral Organics
000423-50-7	423507		Phenols
000429-67-4	429674		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000432-08-6	432086	
	507-63-1	507631	
	000647-42-7	647427	
	000678-26-2	678262	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000432-08-6	N(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	8.72E-04	1.16E-01
507-63-1	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I	F		
000647-42-7	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO	F	9.64E-01	1.29E+02
000678-26-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	6.55E+02	8.73E+04

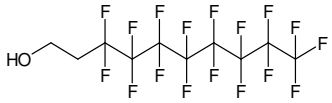
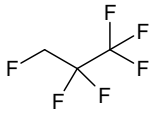
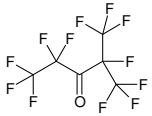
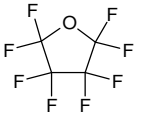
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000432-08-6	a	9.67	15.78	6.11	3	0.500
507-63-1	>100	8.30899E-05	8.77		243.3	2.390
000647-42-7	2.56	0.79	5.60	4.81	4064	3.609
000678-26-2	a	4.16	5.05	0.89	488	2.688

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000432-08-6	see 311897; Persistent; probably amenable to GC-MS analysis	neutral	N	Y	
507-63-1		neutral	N	Y	
000647-42-7	perfluorotelomer - PFHxA precursor?	neutral	N	Y	
000678-26-2	gas GWP concern but not PBT; very volatile but probably amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000432-08-6				N	0.5				
507-63-1		Y	Y	N					No Reports
000647-42-7		PFHxA	Y	N	0.5	0.5		1	1
000678-26-2				N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000432-08-6		Y	1.04E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
507-63-1	10K - 500K		4.02E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000647-42-7		Y	2.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000678-26-2		N	6.20E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000432-08-6	432086		Neutral Organics
507-63-1	507631		halopyridines
000647-42-7	647427		halopyridines
000678-26-2	678262		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000678-39-7	678397	
	000690-39-1	690391	
	000756-13-8	756138	
	000773-14-8	773148	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000678-39-7	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO	F	9.72E-02	1.30E+01
000690-39-1	FC(F)(F)CC(F)(F)F	F	7.02E+03	9.36E+05
000756-13-8	C(C(C(=O)C(C(F)(F)F)(F)C(F)(F)F)(F)F)(F)(F)F	F	9.65E+01	1.29E+04
000773-14-8	O1C(C(C(C1(F)F)(F)F)(F)F)(F)F	f	711	94792.20395

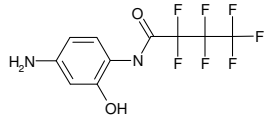
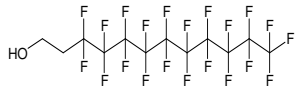
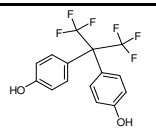
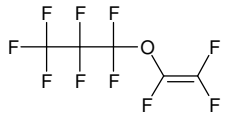
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000678-39-7	2.56	2.23	7.53	5.30	12200	4.086
000690-39-1	2270.91	1.52	2.65	1.13	22	1.337
000756-13-8	a	0.26	2.79	2.53	28	1.448
000773-14-8		-0.072600431	2.14	-1.181686958	8.817	0.945

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000678-39-7	8:2 perfluorotelomer alcohol. Demonstrated to be a PFOA and PFNA	neutral	Y	Y	
000690-39-1	gas GWP concern but not PBT; very volatile but probably amenable to GC analysis	neutral	Y	Y	
000756-13-8	1,1,1,2,2,4,5,5,5-Nonafluoro-4-(trifluoromethyl)-3-pentanone. Referred to as a fire protection fluid. Very volatile but likely amenable to GC-MS analysis	neutral	N	Y	
000773-14-8	P but not B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000678-39-7		PFOA	Y	N	0.5	1			10
000690-39-1				N				0.5	1
000756-13-8				N					0.5
000773-14-8				N					1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000678-39-7		Y	1.21E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000690-39-1		N	5.01E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000756-13-8		Y	6.95E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000773-14-8		Y	30.87	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000678-39-7	678397		amides
000690-39-1	690391		Benzyl Halides
000756-13-8	756138		Esters + Vinyl/Allyl Halides
000773-14-8	773148	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000847-51-8	847518	
	000865-86-1	865861	
	001478-61-1	1478611	
	001623-05-8	1623058	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000847-51-8	O=C(Nc(c(O)cc(N)c1)c1)C(F)(F)C(F)(F)C(F)(F)F	F	2.70E-07	3.60E-05
000865-86-1	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO	F	7.91E-03	1.05E+00
001478-61-1	FC(F)(F)C(c(ccc(O)c1)c1)(c(ccc(O)c2)c2)C(F)(F)F	f	0.00000129	0.000171986
001623-05-8	FC(F)(OC(F)=C(F)F)C(F)(F)C(F)(F)F	F	8.11E+02	1.08E+05

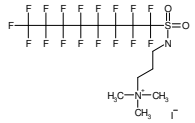
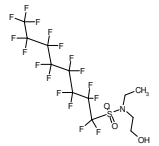
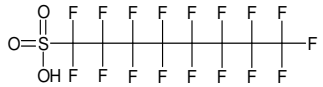
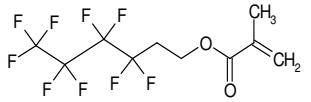
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000847-51-8	0.05	-12.69	2.69	15.38	23	1.369
000865-86-1	2.56	3.67	9.46	5.79	27	1.439
001478-61-1	1.599645041	-7.63422244	4.47	8.709935052	556.3	2.745
001623-05-8	5.79	1.55	3.35	1.80	76	1.878

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000847-51-8	N-(4-amino-2-hydroxyphenyl)-2,2,3,3,4,4,4-heptafluorobutyramide. Likely to yield PFBA on degradation of amide linkage	phenol	N	N	Y
000865-86-1	10:2 fluorotelomer alcohol will degrade to PFDA/PFUnA	neutral	Y	Y	
001478-61-1	Fluorinated Bis-phenol A	phenol	N	N	Y
001623-05-8	Perfluoropropyl vinyl Ether. Very volatile but probably amenable to GC analysis	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000847-51-8		PFBA	Y	N	0.5				
000865-86-1		PFDA	Y	N	0.5	0.5		10	1
001478-61-1				N	0.5	0.5	0.5	0.5	0.5
001623-05-8				N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000847-51-8		Y	14.991	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000865-86-1		N	5.71E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001478-61-1			1.129	Fish 96-hour LC_{50} (mg/L)	
001623-05-8		Y	0.177	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000847-51-8	847518		Aliphatic amine
000865-86-1	865861		Acid Chloride/Halide
001478-61-1	1478611	MPV	Neutral Organics
001623-05-8	1623058		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001652-63-7	1652637	
	001691-99-2	1691992	
	001763-23-1	1763231	
	001799-84-4	1799844	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001652-63-7	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)NCCCN(C)(C)(C)	F	6.17E-09	8.23E-07
001691-99-2	O=S(=O)(N(CCO)CC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.44E-05	3.25E-03
001763-23-1	O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	6.40E-03	8.53E-01
001799-84-4	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(=C)C	f	7.11E+00	9.48E+02

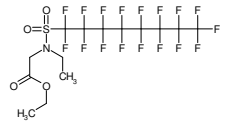
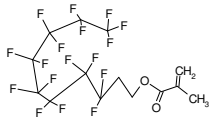
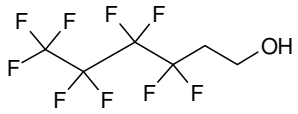
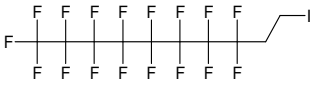
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
001652-63-7	0.40	-7.78	5.27	13.05	6	0.750
001691-99-2	0.45	-1.63	7.78	9.41	5543	3.744
001763-23-1	76.40	-1.35	6.28	7.63	56	1.750
001799-84-4	0.35	1.08	5.57	4.49	3890	3.590

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001652-63-7	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. PFOS degradation product	neutral	N	N	
001691-99-2	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. PFOS degradation product; analysed by GC-MS in air	neutral	Y	Y	
001763-23-1	PFOS	acid	N	N	
001799-84-4	May be analysable with other perfluorotelomers; degrades to perfluorobutanoic acid	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001652-63-7		PFOS	Y	N	0.5				
001691-99-2		PFOS	Y	N	10	10	10	10	0.5
001763-23-1	Y	PFOS	Y	N			0.5		0.5
001799-84-4		PFBuA	Y	N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001652-63-7		Y	1.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001691-99-2		Y	7.27E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001763-23-1		Y	5.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001799-84-4		Y	1.23E-01	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
001652-63-7	1652637		Neutral Organics
001691-99-2	1691992		Acid Chloride/Halide
001763-23-1	1763231		Methacrylates
001799-84-4	1799844		Acrylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001869-77-8	1869778	
	001996-88-9	1996889	
	002043-47-2	2043472	
	002043-53-0	2043530	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001869-77-8	O=C(OCC)CN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)CC	F	2.14E-04	2.85E-02
001996-88-9	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(=C)C	F	1.61E-01	2.15E+01
002043-47-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO	F	9.94E+00	1.33E+03
002043-53-0	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI	F	5.76E-01	7.68E+01

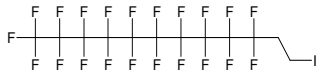
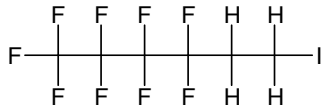
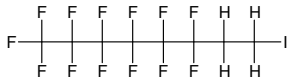
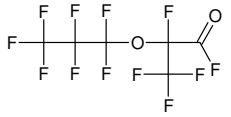
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
001869-77-8	0.81	0.48	8.78	8.30	233	2.366
001996-88-9	0.35	3.96	9.44	5.48	30	1.473
002043-47-2	2.56	-0.65	3.66	4.31	132	2.121
002043-53-0	17.35	4.54	9.75	5.21	11	1.041

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001869-77-8	PFOS related; may be analysable by GC-MS with other perfluorosulamidoalcohols	neutral	N	Y	
001996-88-9	May be analysable with other perfluorotelomers	neutral	N	Y	
002043-47-2	May be analysable with other perfluorotelomers	neutral	N	Y	
002043-53-0	Intermediate for production of perfluorotelomer synthesis	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001869-77-8		PFOS	Y	N	0.5	0.5	0.5	0.5	0.5
001996-88-9		PFOA; PFNA	Y	N	0.5				0.5
002043-47-2		PFBA	Y	N	0.5	0.5		0.5	0.5
002043-53-0		PFOA; PFNA	Y	N		1		10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001869-77-8		N	0.000448	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001996-88-9		N	0.000804	Fish 96-hour LC_{50} (mg/L)	
002043-47-2		Y	4.75E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
002043-53-0		N	2.52E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
001869-77-8	1869778		Dinitrobenzenes
001996-88-9	1996889		Neutral Organics
002043-47-2	2043472		Neutral Organics
002043-53-0	2043530		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002043-54-1	2043541	
	002043-55-2	2043552	
	002043-57-4	2043574	
	002062-98-8	2062988	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002043-54-1	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI	F	9.50E-02	1.27E+01
002043-55-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI	F	1.50E+01	2.00E+03
002043-57-4	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI	F	2.90E+00	3.87E+02
002062-98-8	O=C(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F	F	3.48E+01	4.64E+03

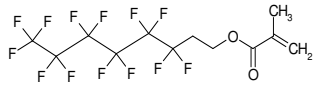
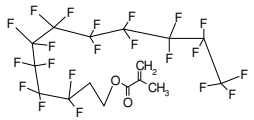
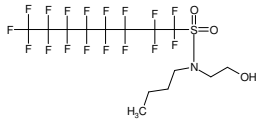
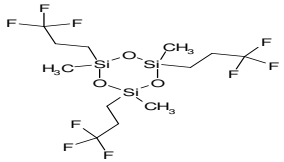
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002043-54-1	17.35	5.98	11.68	5.70	3	0.500
002043-55-2	17.35	1.66	5.89	4.23	6809	3.833
002043-57-4	17.35	3.10	7.82	4.72	4870	3.688
002062-98-8	a	0.38	2.79	2.41	28	1.447

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002043-54-1	Intermediate for production of perfluorotelomer synthesis. Per F = P. May loss iodine. B unknown	neutral	N	N	
002043-55-2	Intermediate for production of perfluorotelomer synthesis	neutral	N	Y	
002043-57-4	Intermediate for production of perfluorotelomer synthesis	neutral	N	Y	
002062-98-8	May be analysable with other perfluorotelomers	acid	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002043-54-1		PFNA;PFDA	Y	N		0.5		1	1
002043-55-2		PFBA	Y	N					
002043-57-4		PFPnA;PFHxA	Y	N	0.5	1		1	10
002062-98-8		PFPrA	Y	N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002043-54-1		N	1.14E-10	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
002043-55-2		N	1.10E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
002043-57-4		N	5.38E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
002062-98-8		Y	2.38E+01	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
002043-54-1	2043541		Acid Chloride/Halide
002043-55-2	2043552		Neutral Organics
002043-57-4	2043574		Neutral Organics
002062-98-8	2062988		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002144-53-8	2144538	
	002144-54-9	2144549	
	002263-09-4	2263094	
Top 10 fluorinated	002374-14-3	2374143	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002144-53-8	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(=C)C	F	1.04E+00	1.39E+02
002144-54-9	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(=C)C	F	1.66E-02	2.21E+00
002263-09-4	O=S(=O)(N(CCCC)CCO)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.65E-06	3.53E-04
002374-14-3	FC(CC[Si]1(O[Si](O[Si](O1)(CCC(F)(F)F)C)(CCC(F)(F)F)C)C)(F)F	F	3.03E-01	4.04E+01

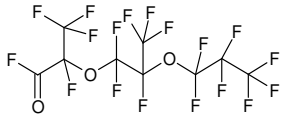
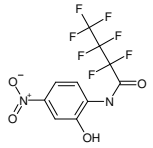
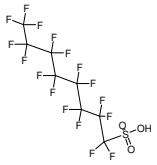
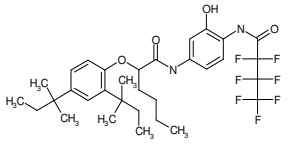
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002144-53-8	0.35	2.52	7.50	4.98	13190	4.120
002144-54-9	0.35	5.40	11.37	5.97	3	0.500
002263-09-4	0.38	-2.38	8.76	11.14	250	2.398
002374-14-3	2.39	3.84	8.66	4.82	343	2.535

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002144-53-8	Per F = P, Acyrlic ester likely to break. May be analysable with other perfluorotelomers	neutral	N	Y	
002144-54-9	Per F = P. Acyrlic ester likely to break. May be analysable with other perfluorotelomers	neutral	N	Y	
002263-09-4	PFOS derivative	neutral	Y	Y	
002374-14-3	Fluorinated cyclic siloxane. May be analysable with other cyclic siloxanes by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002144-53-8		PFPnA;PFHxA	Y	N	0.5	0.5	1	0.5	
002144-54-9		PFNA;PFDA	Y	N	0.5				
002263-09-4		PFOS	Y	N	50	50	50	50	50
002374-14-3				N	10	1	1	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002144-53-8		Y	0.014	Fish 96-hour LC_{50} (mg/L)	
002144-54-9		N	4.55E-05	Fish 96-hour LC_{50} (mg/L)	
002263-09-4		Y	4.55E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	
002374-14-3		N	4.74E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
002144-53-8	2144538		Neutral Organics
002144-54-9	2144549		Neutral Organics
002263-09-4	2263094		Neutral Organics
002374-14-3	2374143		Acid Chloride/Halide

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002641-34-1	2641341	
	002712-83-6	2712836	
	002795-39-3	2795393	
	002923-93-5	2923935	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002641-34-1	O=C(F)C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F)C(F)(F)F	f	8.12E-01	1.08E+02
002712-83-6	O=C(Nc(c(O)cc(N(=O)=O)c1)c1)C(F)(F)C(F)(F)C(F)(F)F	F	1.05E-07	1.40E-05
002795-39-3	S(=O)(=O)(O[K])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	f	5.91E-09	7.88E-07
002923-93-5	O=C(Nc(c(O)cc(NC(=O)C(Oc(c(cc(c1)C(CC)(C)C)C(CC)(C)C)c1)CCCC)c2)c2)C(F)(F)C(F)(F)C(F)(F)F	F	1.86E-17	2.48E-15

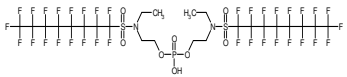
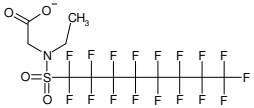
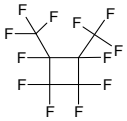
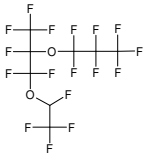
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002641-34-1	a	0.48	4.98	4.50	1363	3.134
002712-83-6	6.43	-11.65	4.72	16.37	856	2.932
002795-39-3	a	-5.85	4.13	9.98	56	1.750
002923-93-5	0.07	-11.94	11.13	23.07	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002641-34-1	Per F = P. Could be B too. Perfluoro(2,5-dimethyl-3,6-dioxananoyl) fluoride. Likely to hydrolyse as carbonyl fluoride. Degradation product could be a PFCA ether	neutral	N	N	
002712-83-6	May degrade to yield PFPrA. Use unknown	phenol	N	N	Y?
002795-39-3	Perfluorooctane sulfonic acid	acid	Y	N	
002923-93-5	Use unknown. Could degrade yielding PFBA	phenol	N	N	Y?

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002641-34-1		PFCA	Y	N				0.5	
002712-83-6		PFPrA	Y	NN	0.5				
002795-39-3	Y	PFOS	Y	Y	0.5	0.5	0.5	0.5	0.5
002923-93-5		PFBA	Y	N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002641-34-1		Y	1.62E+00	Fish 96-hour LC_{50} (mg/L)	
002712-83-6		Y	1.09E+00	Fish 96-hour LC_{50} (mg/L)	Low-moderate
002795-39-3		Y	2.50E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
002923-93-5		Y	2.00E-05	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
002641-34-1	2641341		Methacrylates
002712-83-6	2712836		Neutral Organics
002795-39-3	2795393		Neutral Organics
002923-93-5	2923935		Acid Chloride/Halide

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002965-52-8	2965528	
	002991-51-7	2991517	
	002994-71-0	2994710	
	003330-14-1	3330141	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002965-52-8	O=S(=O)(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)N(CCOP(=O)(OCCN(S(=O)(=O)C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)CC)O)CC	F	1.78E-10	2.37E-08
002991-51-7	[K]OC(=O)CN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	3.65E-11	4.87E-09
002994-71-0	FC(F)(F)C(F)(C(F)(C1(F)F)C(F)(F)F)C1(F)F	f	389	51862.40132
003330-14-1	FC(OC(F)(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F)C(F)(F)F	F	1.54E+01	2.05E+03

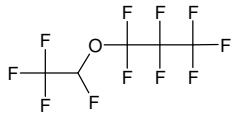
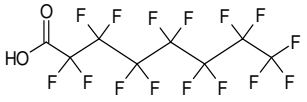
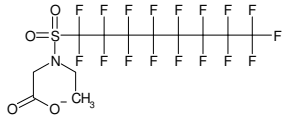
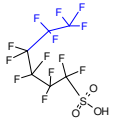
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002965-52-8	0.16	-3.84	16.16	20.00	3	0.500
002991-51-7	0.93	-7.38	4.20	11.58	10	1.000
002994-71-0		4.923183085	3.72	-4.597470473	145	2.161
003330-14-1	4129.73	1.31	5.93	4.62	7355	3.867

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002965-52-8	1-Octanesulfonamide,. N,N'-[phosphinicobis(oxy-2,1-ethanediyl)]bis[N-ethyl-. 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-. PFOS - phosphate based product. Likely phased out with phase out of PFOS based chemistry in 2001	neutral	N	N	
002991-51-7	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. Carboyxlate group may make it amenable to LC-MS analysis	acid	N	N	
002994-71-0	Per F = P. Very volatile. GWP chem. Not B	neutral	N	Y	
003330-14-1	2H-Perfluoro(5-methyl-3,6-dioxanonane. Refrigerant. Analysable by GC-MS suitably modified for gas analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002965-52-8	Y?	PFOS	Y	N			0.5	0.5	
002991-51-7	Y	PFOS	Y	N	0.5	0.5	0.5	0.5	
002994-71-0				N			0.5		
003330-14-1				N			0.5		0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002965-52-8		Y	5.14E-16	Mysid Shrimp 96-hour LC_{50} (mg/L)	
002991-51-7		Y	2.37E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
002994-71-0			2.095	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003330-14-1		Y	1.18E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
002965-52-8	2965528		Neutral Organics
002991-51-7	2991517		Acid Chloride/Halide
002994-71-0	2994710	MPV	Neutral Organics
003330-14-1	3330141		Acrylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	003330-15-2	3330152	
	003825-26-1	3825261	
Top 10 chlorinated	003871-50-9	3871509	
	003871-99-6	3871996	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
003330-15-2	FC(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F	F	4.27E+02	5.69E+04
003825-26-1	N(H)(H)(H)OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	7.14E-05	9.52E-03
003871-50-9	[Na]OC(=O)CN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	3.65E-11	4.87E-09
003871-99-6	S(=O)(=O)(O[K])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	f	8.12E-09	1.08E-06

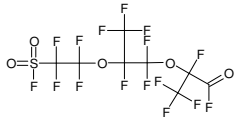
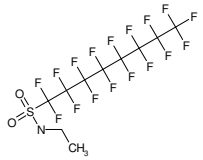
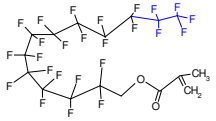
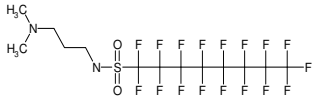
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
003330-15-2	4129.73	1.20	3.74	2.54	151	2.179
003825-26-1	a	-7.75	3.42	11.17	3	0.500
003871-50-9	0.93	-2.14	4.20	6.34	10	1.000
003871-99-6	a	-8.09	2.20	10.29	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
003330-15-2	Fluoroether. Cleaning solvent and blowing agents. GW potential. Could be analysable by GC modified for gas analysis	neutral	N	Y	
003825-26-1	Perfluorooctanoic acid	acid	Y	Y	
003871-50-9	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. Carboxylate group may make it amenable to LC-MS analysis	acid	N	N	
003871-99-6	Perfluorohexanesulfonic acid	acid	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
003330-15-2				N			0.5		
003825-26-1	Y	PFOA	Y	Y	0.5	0.5	0.5	0.5	1
003871-50-9	Y	PFOS	Y	N	0.5	0.5			
003871-99-6		PFHxS	Y	Y		0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
003330-15-2		Y	4.09E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003825-26-1		Y	1.55E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003871-50-9		Y	2.31E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003871-99-6		Y	5.27E+01	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
003330-15-2	3330152		Vinyl/Allyl Ethers
003825-26-1	3825261		Neutral Organics
003871-50-9	3871509		Neutral Organics
003871-99-6	3871996		amides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	004089-58-1	4089581	
	004151-50-2	4151502	
	006014-75-1	6014751	
	013417-01-1	13417011	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
004089-58-1	O=C(F)C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)F)C(F)(F)F	f	0.0221	2.946424342
004151-50-2	O=S(=O)(NCC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	f	8.24E-02	1.10E+01
006014-75-1	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(=C)C	F	1.92E-03	2.56E-01
013417-01-1	O=S(=O)(NCCCN(C)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	7.97E-04	1.06E-01

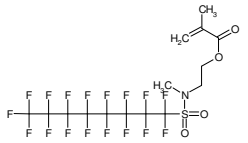
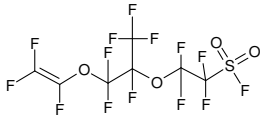
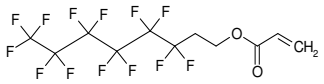
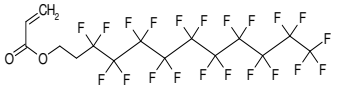
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
004089-58-1		-2.510623824	5.68	4.796336436	4709	3.673
004151-50-2	1.21	2.34	8.54	6.20	500	2.699
006014-75-1	0.35	6.84	13.30	6.46	3	0.500
013417-01-1	0.42	-1.84	8.24	10.08	1300	3.114

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
004089-58-1	Per F = P and possibly B	acid	N	N	
004151-50-2	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. Analysable with other perfluoroalkylsulfonamides by GC-MS	neutral	Y	Y	
006014-75-1	2-Propenoic acid, 2-methyl-, 3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl ester. Acrylate for use in fluoropolymers. May be amenable to GC-MS analysis	neutral	N	Y	
013417-01-1	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
004089-58-1		perfluoroalkyl ether	Y?	N	0.5		0.5	0.5	0.5
004151-50-2		PFOS	Y	N			0.5	0.5	0.5
006014-75-1		PFDoA	Y	N	0.5				
013417-01-1		PFOS	Y	N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
004089-58-1			0.514	Fish 96-hour LC_{50} (mg/L)	
004151-50-2		Y	7.53E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	
006014-75-1		N	2.51E-06	Fish 96-hour LC_{50} (mg/L)	
013417-01-1		Y	0.005	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
004089-58-1	4089581	MPV	Acrylates
004151-50-2	4151502		Thiols(mercaptans)
006014-75-1	6014751		Neutral Organics
013417-01-1	13417011		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	014650-24-9	14650249	
	016090-14-5	16090145	
	017527-29-6	17527296	
	017741-60-5	17741605	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
014650-24-9	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C)C(=C)C	F	1.22E-04	1.63E-02
016090-14-5	O=S(=O)(F)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)=C(F)F	F	1.60E-01	2.13E+01
017527-29-6	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C=C	F	2.18E+00	2.91E+02
017741-60-5	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C=C	F	3.39E-02	4.52E+00

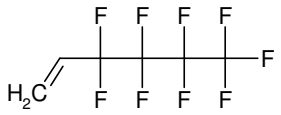
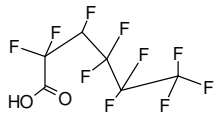
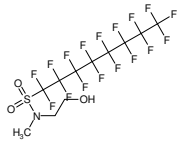
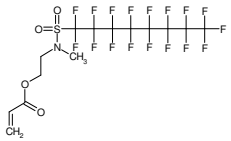
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
014650-24-9	0.25	-1.02	9.19	10.21	64	1.803
016090-14-5	5.79	-2.34	6.24	8.58	12710	4.104
017527-29-6	0.84	2.32	6.96	4.64	45320	4.656
017741-60-5	0.84	5.20	10.82	5.62	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
014650-24-9	Perfluorooctananesulfonamide related. Acrylate for use in fluoropolymers. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y?	
016090-14-5	Perfluorosulfonyl fluoride. Used as an intermediate in perfluoro chemical synthesis. Should yield sulfonate on reaction with water	acid	N	N	
017527-29-6	Acrylate of perfluorotelomer. May degrade to PFHxA or PFPnA. May be amenable to GC analysis	neutral	N	Y	
017741-60-5	Acrylate of perfluorotelomer. May degrade to PFNA or PFDA. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
014650-24-9		PFOS	Y	N	0.5	0.5	0.5	0.5	
016090-14-5		Perfluoroalkyl ether sulfonate	Y	N	0.5		0.5	0.5	0.5
017527-29-6		PFHxA/PFPnA	Y	N		0.5		0.5	0.5
017741-60-5		PFNA/PFDA	Y	N		0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
014650-24-9		N	0.00138	Fish 96-hour LC_{50} (mg/L)	
016090-14-5		Y	0.239	Fish 96-hour LC_{50} (mg/L)	
017527-29-6		Y	0.02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
017741-60-5		N	0.064	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
014650-24-9			Neutral Organics
016090-14-5			Neutral Organics
017527-29-6			Aliphatic amine
017741-60-5			Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	019430-93-4	19430934	
	021615-47-4	21615474	
	024448-09-7	24448097	
	025268-77-3	25268773	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
019430-93-4	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C=C	F	1.38E+03	1.84E+05
021615-47-4	N(H)(H)(H)OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.17E-04	1.56E-02
024448-09-7	O=S(=O)(N(CCO)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	8.04E-05	1.07E-02
025268-77-3	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C)C=C	F	2.31E-04	3.08E-02

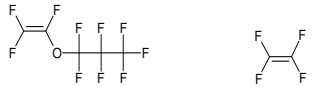
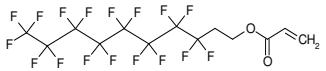
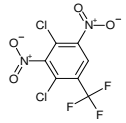
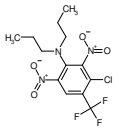
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
019430-93-4	0.49	2.66	4.99	2.33	1393	3.144
021615-47-4		-9.19	1.49	10.68	3	0.500
024448-09-7	0.66	-1.75	7.29	9.04	26090	4.416
025268-77-3	0.43	-1.22	8.65	9.87	357	2.553

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
019430-93-4	Intermediate in fluoropolymer production? Very volatile. Amendable to GC analysis. May degrade to PFPnA	neutral	N	Y	
021615-47-4	Ammonium salt of PFHxA	acid	Y	N	
024448-09-7	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	
025268-77-3	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. Acrylate may be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
019430-93-4		PFPnA	Y	N	0.5	0.5		0.5	0.5
021615-47-4	Y	PFPnA	Y	Y			0.5	0.5	
024448-09-7		PFOS	Y	N	1	10	10	10	
025268-77-3		PFOS	Y	N	1	1	1	1	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
019430-93-4		N	1.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
021615-47-4		Y	715.521	Fish 96-hour LC_{50} (mg/L)	
024448-09-7		Y	2.91E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
025268-77-3		Y	0.006	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
019430-93-4			Aliphatic amine
021615-47-4			Neutral Organics
024448-09-7			Neutral Organics
025268-77-3			Esters + Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	026655-00-5	26655005	
	027905-45-9	27905459	
	029091-09-6	29091096	
Top 10 fluorinated	029091-20-1	29091201	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
026655-00-5	F/C(F)=C(F)\OC(F)(F)C(F)(F)C(F)(F)F	F	8.11E+02	1.08E+05
027905-45-9	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C=C	F	3.29E-01	4.39E+01
029091-09-6	O=N(=O)c(c(c(N(=O)=O)c(c1C(F)(F)F)Cl)Cl)c1	f	0.0000272	0.003626368
029091-20-1	N(=O)(=O)c1c(c(c(c(c1)C(F)(F)F)Cl)N(=O)(=O))N(CCC)CCC	f	0.000000352	4.69295E-05

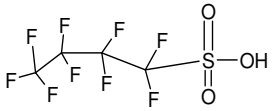
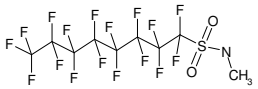
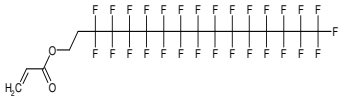
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
026655-00-5	8.08	2.55	3.35	0.80	76	1.878
027905-45-9	0.84	3.76	8.89	5.13	167	2.223
029091-09-6	675582.0473	-4.786510785	3.88	5.272223396	194	2.288
029091-20-1	5.348061503	-2.192671124	5.96	4.758383735	7688	3.886

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
026655-00-5	May be amenable to GC analysis. Degradation product could be PFPrA?	neutral	N	Y	
027905-45-9	Acrylate of perfluorotelomer. May degrade to PFOA or PFHpA. May be amenable to GC analysis	neutral	N	Y	
029091-09-6	Very P but not B. Uses?	neutral	N	Y	
029091-20-1	P & B Dinitroamine pesticide??	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
026655-00-5		PFPrA?	Y	N		0.5		0.5	
027905-45-9		PFOA	Y	N		0.5		0.5	1
029091-09-6				N	0.5		1	1	
029091-20-1				N	0.5		1	1	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
026655-00-5		Y	0.158	Fish 96-hour LC_{50} (mg/L)	
027905-45-9		Y	0.004	Mysid Shrimp 96-hour LC_{50} (mg/L)	
029091-09-6			0.55	Fish 96-hour LC_{50} (mg/L)	Low-moderate
029091-20-1			0.031	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
026655-00-5			amine
027905-45-9			Neutral Organics
029091-09-6	29091096	MPV	Neutral Organics
029091-20-1	29091201	MPV	Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	029420-49-3	29420493	
	030046-31-2	30046312	
	031506-32-8	31506328	
	034362-49-7	34362497	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
029420-49-3	S(=O)(=O)(O[K])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.12E-08	1.49E-06
030046-31-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI	F	1.33E-02	1.77E+00
031506-32-8	O=S(=O)(NC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	f	2.68E-01	3.57E+01
034362-49-7	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C=C	F	5.87E-04	7.83E-02

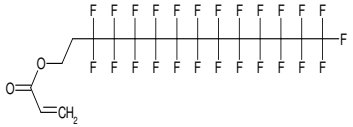
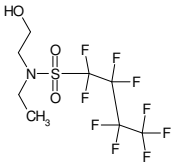
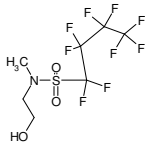
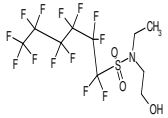
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
029420-49-3		-10.33	0.26	10.59	3	0.500
030046-31-2	17.35	7.42	13.62	6.20	3	0.500
031506-32-8	8.46	2.22	8.05	5.83	2355	3.372
034362-49-7	0.84	7.09	14.68	7.59	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
029420-49-3	Perfluorobutanesulfonate (PFBS)	acid	Y	Y	
030046-31-2	Perfluorotelomer iodide intermediate. May degrade to C11 or C12 PFCA.	neutral	N	N	
031506-32-8	Perfluorooctananesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	Y	Y	
034362-49-7	Acrylate of perfluorotelomer. May degrade to C13 or C14 PFCA. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
029420-49-3	Y	PFBS	Y	Y	0.5	0.5	0.5	0.5	0.5
030046-31-2		PFDoA	Y	N		0.5		0.5	0.5
031506-32-8		PFOS	Y	N	0.5		0.5	0.5	0.5
034362-49-7		PFTrDA	Y	N		0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
029420-49-3		Y	8776.035	Fish 96-hour LC_{50} (mg/L)	
030046-31-2		N	4.94E-13	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
031506-32-8		N	3.00E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
034362-49-7		N	2.32E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
029420-49-3			Neutral Organics
030046-31-2			Anilines (amino-meta) + Triazines
031506-32-8			Imides
034362-49-7	34362497		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	034395-24-9	34395249	
	034449-89-3	34449893	
	034454-97-2	34454972	
	034455-03-3	34455033	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
034395-24-9	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C=C	F	4.46E-03	5.95E-01
034449-89-3	O=S(=O)(N(CCO)CC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	8.36E-05	1.11E-02
034454-97-2	O=S(=O)(N(CCO)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.86E-04	3.81E-02
034455-03-3	O=S(=O)(N(CCO)CC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	4.50E-05	6.00E-03

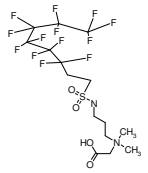
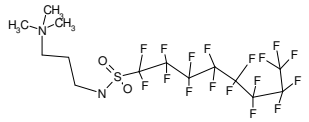
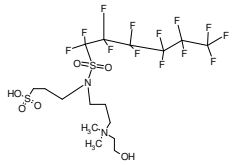
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
034395-24-9	0.84	5.65	12.75	7.11	3	0.500
034449-89-3	0.45	-4.51	3.91	8.42	206	2.314
034454-97-2	0.66	-4.64	3.42	8.06	86	1.936
034455-03-3	0.45	-3.07	5.85	8.92	6331	3.801

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
034395-24-9	Acrylate of perfluorotelomer. May degrade to C11 or C11 PFCA. May be amenable to GC analysis	neutral	N	Y	
034449-89-3	Perfluorobutanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	
034454-97-2	Perfluorobutanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	
034455-03-3	Perfluorohexanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis.' Per F = P C4 metabolite, air breathing biomagnification	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
034395-24-9		PFDoA	Y	N		0.5		0.5	0.5
034449-89-3		PFBS	Y	N	0.5	0.5	0.5	0.5	
034454-97-2		PFBS	Y	N	0.5	0.5	0.5	0.5	0.5
034455-03-3		PFHxS	Y	N	0.5	0.5	0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
034395-24-9		N	0.00013	Mysid Shrimp 96-hour LC_{50} (mg/L)	
034449-89-3		Y	3.25E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
034454-97-2		Y	1.28E+00	Mysid Shrimp 96-hour LC_{50} (mg/L)	
034455-03-3		Y	1.55E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
034395-24-9	34395249		Dinitrobenzenes
034449-89-3	34449893		Neutral Organics
034454-97-2	34454972		Dinitrobenzenes
034455-03-3	34455033		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	034455-29-3	34455293	
	038006-74-5	38006745	
	038850-58-7	38850587	
	039239-77-5	39239775	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
034455-29-3	O=C(O1)CN1(CCCNS(=O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)(C)C	F	3.91E-12	5.21E-10
038006-74-5	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)NCCCN(C)(C)(C)	F	6.17E-09	8.23E-07
038850-58-7	O=S(=O)(N(CCCN(CCO)(C)C)CCCS(=O)(=O)O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.91E-19	3.88E-17
039239-77-5	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO	F	6.01E-04	8.01E-02

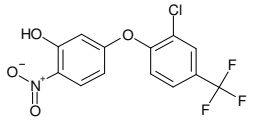
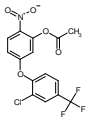
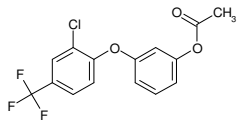
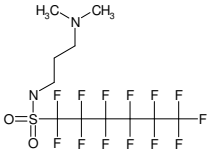
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
034455-29-3	0.31	-10.32	1.51	11.83	3	0.500
038006-74-5	0.40	-7.78	5.27	13.05	6	0.750
038850-58-7	0.20	-19.72	0.34	20.06	3	0.500
039239-77-5	2.56	5.11	11.39	6.28	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
034455-29-3	Fluorotelomer sulfonate related compound. Likely to degrade to PFHxA. May be amenable to LC-MS analysis as carboxylate	acid	N	Y	
038006-74-5	PFOS related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	
038850-58-7	Perfluorohexanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	acid	N	Y	
039239-77-5	Fluorotelomer alcohol. May degrade to C11 or C12 PFCA. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
034455-29-3		PFHxA	Y	N	0.5				
038006-74-5		PFOS	Y	N	0.5	0.5	0.5	0.5	
038850-58-7		PFHxS	Y	N	0.5	1	0.5		
039239-77-5		PFDoA	Y	N	0.5	0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
034455-29-3		Y	179.461	Fish 96-hour LC_{50} (mg/L)	
038006-74-5		Y	1.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
038850-58-7		Y	17214.021	Fish 96-hour LC_{50} (mg/L)	
039239-77-5		N	2.60E-10	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
034455-29-3	34455293		Neutral Organics
038006-74-5	38006745		Dinitrobenzenes
038850-58-7	38850587		Dinitrobenzenes
039239-77-5	39239775		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	042874-63-5	42874635	
	050594-44-0	50594440	
Top 10 brominated	050594-77-9	50594779	
	050598-28-2	50598282	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
042874-63-5	O=N(=O)c(c(O)cc(Oc(c(cc(c1)C(F)(F)F)Cl)c1)c2)c2	F	8.72E-08	1.16E-05
050594-44-0	O=C(Oc(c(N(=O)=O)ccc1Oc(c(cc(c2)C(F)(F)F)Cl)c2)c1)C	f	0.000000166	2.21315E-05
050594-77-9	O=C(Oc(cc(Oc(c(cc(c1)C(F)(F)F)Cl)c1)cc2)c2)C	F	1.41E-05	1.88E-03
050598-28-2	O=S(=O)(NCCCN(C)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.40E-03	1.87E-01

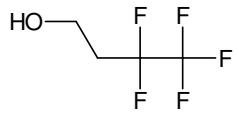
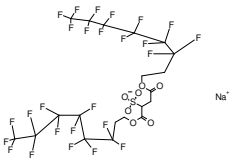
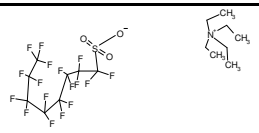
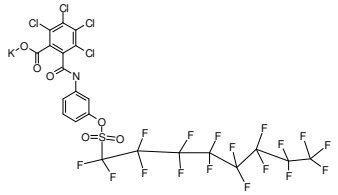
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
042874-63-5	1.29	-5.40	4.73	10.13	879	2.944
050594-44-0	173.1443839	-5.832268275	4.23	6.667980887	361.8	2.558
050594-77-9	2.56	-3.43	4.41	7.84	500	2.699
050598-28-2	0.42	-3.28	6.31	9.59	14300	4.155

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
042874-63-5	Process intermediate. Likely persistent. Might be a pesticide intermediate. Could yield phenolic degradation product	phenol	N	N	Y
050594-44-0	Ester will hydrolysis rapidly (LOGKOW of phenol ~4.34, persistent metabolites?	neutral	N	Y	
050594-77-9	Intermediate in pesticide production. Ester will hydrolyse rapidly (LOGKOW of phenol 4.34, persistent metabolites? Could be amenable to GC anlaysis or as phenolic degradation product	neutral	N	Y	
050598-28-2	Perfluorohexanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
042874-63-5		halogenated diphenyl(ol)	Y	N			0.5	1	10
050594-44-0				N	1	10	10		
050594-77-9		halogenated diphenyl(ol)	Y	N	1	10		10	10
050598-28-2		PFHxS	Y	N		0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
042874-63-5		Y	1.02E+00	Fish 96-hour LC_{50} (mg/L)	
050594-44-0			1.206	Mysid Shrimp 96-hour LC_{50} (mg/L)	
050594-77-9		Y	0.759	Mysid Shrimp 96-hour LC_{50} (mg/L)	
050598-28-2		N	0.046	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
042874-63-5	42874635		Phenols
050594-44-0	50594440	airbreather	Neutral Organics
050594-77-9	50594779		Neutral Organics
050598-28-2	50598282		Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	054949-74-5	54949745	
	054950-05-9	54950059	
	056773-42-3	56773423	
	057589-85-2	57589852	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
054949-74-5	FC(F)(F)C(F)(F)CCO	F	6.33E+01	8.44E+03
054950-05-9	O=C(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(S(=O)([O-])=O)CC(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)=O.[Na+]	F	4.78E-13	6.37E-11
056773-42-3	O=S(=O)(ON(CC)(CC)(CC)CC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	f	2.57E-09	3.42638E-07
057589-85-2	O=S(=O)(Oc2cccc(c2)NC(=O)c1c(c(c(c(c1Cl)Cl)Cl)Cl)C(=O)O[K])C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	3.62E-21	4.83E-19

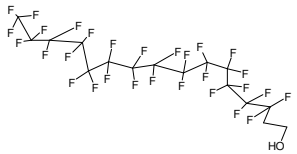
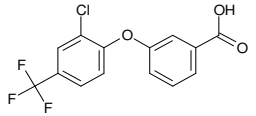
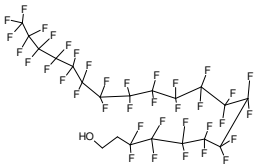
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
054949-74-5	2.56	-3.10	1.73	4.83	4	0.633
054950-05-9	2.22	-2.92	9.68	12.60	3	0.500
056773-42-3	3.62458008	-7.143058108	9.14	12.88877072	3.162	0.500
057589-85-2	0.08	-11.13	9.03	20.16	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
054949-74-5	Fluorotelomer alcohol - may degrade to PFPrA. Very volatile but possibly analysable with other longer chain fluorotelomer alcohols	neutral	N	Y	
054950-05-9	Fluorotelomer sulfonate related compound. Likely to degrade to PFHxA. May be amenable to LC-MS analysis as sulfate	neutral	N	N	
056773-42-3	Per F = P PFOA precursor	acid	Y	N	
057589-85-2	PFOS related compound. Likely to degrade to PFOS	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
054949-74-5		PFPrA	Y	N	0.5				
054950-05-9	Y	PFHxA	Y	N				0.5	
056773-42-3	Y	PFOS	Y	Y				0.5	0.5
057589-85-2		PFOS	Y	N	0.5	0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
054949-74-5		Y	217.782	Fish 96-hour LC_{50} (mg/L)	
054950-05-9		Y	1.00E-02	Fish 96-hour LC_{50} (mg/L)	
056773-42-3		Y	1.56E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
057589-85-2		Y	0.000425	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
054949-74-5	54949745		Phenols
054950-05-9	54950059		Phenols
056773-42-3	56773423	MPV	Benzotriazoles + Phenols
057589-85-2	57589852		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	060699-51-6	60699516	
	063734-62-3	63734623	
	065104-63-4	65104634	
	065104-65-6	65104656	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
060699-51-6	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCO	F	6.44E-05	8.59E-03
063734-62-3	O=C(O)c(cc(Oc(c(cc(c1)C(F)(F)F)Cl)c1)cc2)c2	f	0.000000996	0.000132789
065104-63-4	FC(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(CCl)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)F	F	1.11E-04	1.48E-02
065104-65-6	FC(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(C(C(CCO)(F)F)(F)F)(F)F)F	F	1.15E-06	1.53E-04

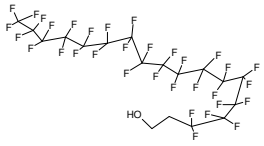
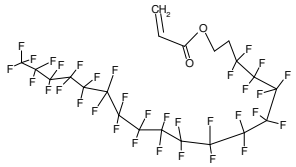
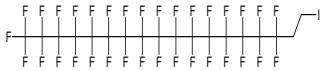
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
060699-51-6	2.56	6.55	13.32	6.77	3	0.500
063734-62-3	70.31068294	-6.203879345	4.7	7.509591957	3.162	0.500
065104-63-4	17.35	11.75	19.41	7.66	3	0.500
065104-65-6	2.56	9.43	17.19	7.76	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
060699-51-6	Fluorotelomer alcohol. May degrade to C13 or C14 PFCA. May be amenable to GC analysis	neutral	N	Y	
063734-62-3	P - especially the CF3 ring, pKa important. No production anymore?	acid	N	N	Y
065104-63-4	Fluorotelomer iodide intermediate. May degrade to C17 or C18 PFCA.	neutral	N	N	
065104-65-6	Fluorotelomer alcohol. May degrade to C17 or C18 PFCA. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
060699-51-6		PFTrDA	Y	N	1			0.5	0.5
063734-62-3	Y	carboxylate	Y	N	10	10	10		
065104-63-4		PFC(18)	Y	N	0.5				
065104-65-6		PFC(18)	Y	N	0.5	0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
060699-51-6		N	1.16E-12	Mysid Shrimp 96-hour LC_{50} (mg/L)	
063734-62-3			1.499	Mysid Shrimp 96-hour LC_{50} (mg/L)	
065104-63-4		N	3.97E-20	Mysid Shrimp 96-hour LC_{50} (mg/L)	
065104-65-6		N	2.12E-17	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
060699-51-6	60699516		Neutral Organics
063734-62-3	63734623	airbreather	Neutral Organics
065104-63-4	65104634		Aliphatic amine
065104-65-6	65104656		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	065104-67-8	65104678	
	065150-93-8	65150938	
	065150-94-9	65150949	
	065510-55-6	65510556	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
065104-67-8	FC(C(C(C(C(C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(C(C(CCO)(F)F)(F)F)(F)F)F	F	7.19E-06	9.59E-04
065150-93-8	C=CC(OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)=O	F	9.02E-05	1.20E-02
065150-94-9	FC(C(C(C(C(C(C(C(C(C(C(C(C(CCI)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)F	F	4.54E-04	6.05E-02
065510-55-6	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI	F	2.50E-03	3.33E-01

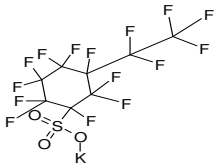
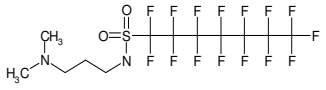
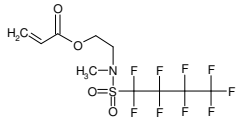
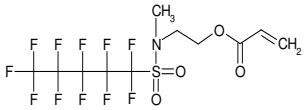
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
065104-67-8	2.56	7.99	15.26	7.27	3	0.500
065150-93-8	0.84	8.53	16.62	8.09	3	0.500
065150-94-9	17.35	10.30	17.48	7.18	3	0.500
065510-55-6	17.35	8.86	15.55	6.69	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
065104-67-8	Fluorotelomer alcohol. May degrade to C15 or C16 PFCA. May be amenable to GC analysis	neutral	N	Y	
065150-93-8	Acrylate of perfluorotelomer. May degrade to C15 or C16 PFCA	neutral	N	N	
065150-94-9	May degrade to C15 or C16 PFCA	neutral	N	N	
065510-55-6	May degrade to C13 or C14 PFCA	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
065104-67-8		PFC(16)	Y	N				0.5	0.5
065150-93-8		PFC(16)	Y	N	10	0.5		0.5	0.5
065150-94-9		PFC(16)	Y	N		0.5		0.5	0.5
065510-55-6		PFTrDA	Y	N	0.5	0.5			0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
065104-67-8		N	4.92E-15	Mysid Shrimp 96-hour LC_{50} (mg/L)	
065150-93-8		N	3.20E-02	Fish 96-hour LC_{50} (mg/L)	
065150-94-9		N	9.30E-18	Mysid Shrimp 96-hour LC_{50} (mg/L)	
065510-55-6		N	2.16E-15	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
065104-67-8	65104678		Neutral Organics
065150-93-8	65150938		amine
065150-94-9	65150949		Amides Acid
065510-55-6	65510556		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 fluorinated	067584-42-3	67584423	
	067584-54-7	67584547	
	067584-55-8	67584558	
	067584-56-9	67584569	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
067584-42-3	O=S(=O)(C1(C(C(C(C(C1(F)F)(C(C(F)(F)F)(F)F)F)(F)F)(F)F)(F)F)F)O[K]	F	1.57E-09	2.09E-07
067584-54-7	O=S(=O)(NCCCN(C)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.06E-03	1.41E-01
067584-55-8	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C)C=C	F	6.87E-04	9.16E-02
067584-56-9	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C)C=C	F	5.22E-04	6.96E-02

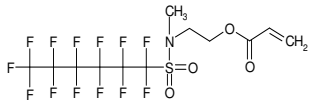
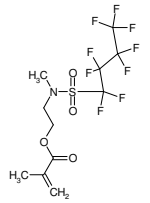
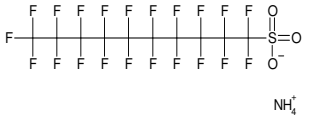
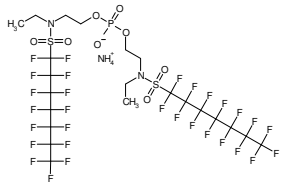
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
067584-42-3	a	-9.83	0.47	10.30	3	0.500
067584-54-7	0.42	-2.56	7.27	9.83	27380	4.437
067584-55-8	0.43	-4.10	4.78	8.88	961	2.983
067584-56-9	0.43	-3.38	5.75	9.13	5330	3.727

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
067584-42-3	May be analysable along with other perfluoroalkane sulfonates. See precursor 68156-06-9	acid	N	N	
067584-54-7	Perfluoroheptanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	
067584-55-8	Perfluorobutanesulfonamide related. May be amenable to GC analysis	neutral	N	Y	
067584-56-9	Perfluoropentanesulfonamide related. May be related to Perfluorobutanesulfonatechemistry. May be amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
067584-42-3	Y			Y			0.5	0.5	
067584-54-7		PFHpS	Y	N	0.5	0.5	0.5	0.5	
067584-55-8		PFBS	Y	N		0.5	0.5		
067584-56-9		PFPnS	Y	N	0.5	0.5	0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
067584-42-3		Y	165	Mysid Shrimp 96-hour LC_{50} (mg/L)	
067584-54-7		Y	0.063	Fish 96-hour LC_{50} (mg/L)	
067584-55-8		Y	1.24	Fish 96-hour LC_{50} (mg/L)	
067584-56-9		Y	0.811	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
067584-42-3	67584423		Neutral organics-Acid
067584-54-7	67584547		Neutral Organics
067584-55-8	67584558		Neutral Organics
067584-56-9	67584569		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	067584-57-0	67584570	
	67584-59-2	67584592	
	067906-42-7	67906427	
	067939-97-3	67939973	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
067584-57-0	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C)C=C	F	3.98E-04	5.31E-02
67584-59-2	C=C(C)C(=O)OCCN(C)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F		
067906-42-7	S(=O)(=O)(ON(H)(H)(H)H)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	8.43E-07	1.12E-04
067939-97-3	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)N(CC)CCOP(=O)(ON(H)(H)(H)H)OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.06E-08	2.75E-06

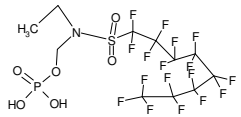
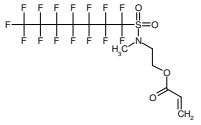
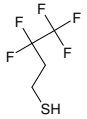
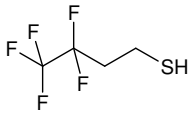
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
067584-57-0	0.43	-2.66	6.72	9.38	29550	4.471
67584-59-2	1.01	0.00124	5.33		2537	3.400
067906-42-7		-7.22	8.92	16.14	10	1.000
067939-97-3	0.12	-12.60	10.89	23.49	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
067584-57-0	Perfluorohexanesulfonamide related. Phased out with PFOS related chemistry. May be amenable to GC analysis	neutral	N	Y	
67584-59-2	Acrylate of perfluorobutanesulfonamide - replacement for PFOS related chemicals	neutral	Y	N	
067906-42-7	PFDS - ammonium salt	neutral	Y	N	
067939-97-3	Perfluorosulfonamido-phosphate derivative. Chemistry may have been phased out in 2001 with phase out of PFOS	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
067584-57-0		PFHxS	Y	N		0.5	0.5	0.5	0.5
67584-59-2		Y	Y	N					No Reports
067906-42-7	Y	PFDS		Y			0.5		
067939-97-3	Y	PFHpS	Y	N			0.5		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
067584-57-0		Y	0.524	Fish 96-hour LC_{50} (mg/L)	
67584-59-2	10K - 500K		0.127	Fish 96-hour LC_{50} (mg/L)	
067906-42-7		Y	2.95E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	
067939-97-3		Y	1.85E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
067584-57-0	67584570		amine
67584-59-2	67584592		Neutral Organics
067906-42-7	67906427		Benzotriazoles + Phenols
067939-97-3	67939973		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	067969-69-1	67969691	
	068084-62-8	68084628	
	068140-18-1	68140181	
	068140-19-2	68140192	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
067969-69-1	N(H)(H)(H)OP(ON(H)(H)(H)H)(=O)OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.06E-08	2.75E-06
068084-62-8	O=C(OCCN(S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C)C=C	F	3.03E-04	4.04E-02
068140-18-1	FC(C(CCS)(F)F)(F)F	F	1.29E+02	1.72E+04
068140-19-2	FC(C(CCS)(F)F)(F)F	F	1.29E+02	1.72E+04

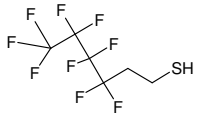
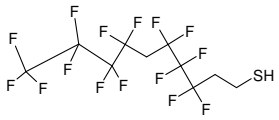
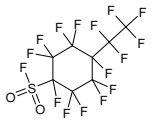
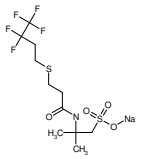
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
067969-69-1	0.25	-18.31	5.61	23.92	6	0.750
068084-62-8	0.43	-1.94	7.68	9.62	7529	3.877
068140-18-1	0.26	-0.11	3.14	3.25	52	1.718
068140-19-2	0.26	-0.11	3.14	3.25	52	1.718

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
067969-69-1	Perfluorosulfonamido-phosphate derivative. Chemistry may have been phased out in 2001 with phase out of PFOS	neutral	N	N	
068084-62-8	Perfluorosulfonamido-alcohol derivative. Chemistry may have been phased out in 2001 with phase out of PFOS	neutral	N	Y	
068140-18-1	Perfluoroteomer derivative? May degrade to perfluoropropionic acid	neutral	N	Y?	
068140-19-2	Perfluorotelomer derivative? May degrade to perfluoropropionic acid	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
067969-69-1	Y?	PFOS	Y	N		0.5			
068084-62-8		PFHpS	Y	N	0.5	0.5	0.5	0.5	
068140-18-1		PFPrA	Y	N	0.5	0.5	0.5	0.5	
068140-19-2		PFPrA	Y	N	0.5	0.5	0.5	1	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
067969-69-1		Y	5.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068084-62-8		Y	0.335	Fish 96-hour LC_{50} (mg/L)	
068140-18-1		Y	0.932	Fish 96-hour LC_{50} (mg/L)	
068140-19-2		Y	0.932	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
067969-69-1	67969691		Neutral Organics
068084-62-8	68084628		Esters
068140-18-1	68140181		Imides + Phenols
068140-19-2	68140192		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068140-20-5	68140205	
	068140-21-6	68140216	
	068156-06-9	68156069	
	068187-47-3	68187473	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068140-20-5	FC(C(CCS)(F)F)(F)C(C(F)(F)F)(F)F	F	8.63E+01	1.15E+04
068140-21-6	FC(C(CCS)(F)F)(F)C(CC(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F	F	1.67E+01	2.23E+03
068156-06-9	O=S(=O)(C1(C(C(F)(F)C(C(C1(F)F)(F)F)(C(C(F)(F)F)(F)F)(F)F)F)F	F	7.99E-01	1.07E+02
068187-47-3	CC(C)(NC(=O)CCSCCC(F)(F)C(F)(F)(F))CS(=O)(=O)O[Na]	F	1.62E-15	2.16E-13

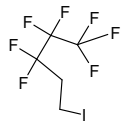
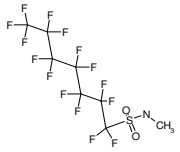
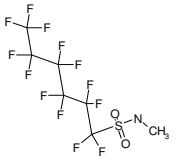
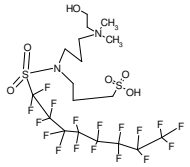
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
068140-20-5	0.26	1.33	5.07	3.74	1606	3.206
068140-21-6	0.26	3.62	8.46	4.84	642	2.807
068156-06-9		1.49	5.96	4.47	7741	3.889
068187-47-3	0.26	-12.38	-1.75	10.63	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068140-20-5	Perfluorotelomer derivative? May degrade to perfluoropentanoic acid	neutral	N	Y?	
068140-21-6	Perfluorotelomer derivative? May degrade to perfluorocarboyxylate	neutral	N	Y?	
068156-06-9	May hydrolyse to a perfluorosulfonic acid	acid	N	N	
068187-47-3	Perfluoroteomer derivative? May degrade to perfluoropropionic acid	acid	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068140-20-5		PFPnA	Y	N	0.5	0.5	0.5	0.5	
068140-21-6		PFCA?	Y	N	0.5	0.5	0.5	0.5	
068156-06-9		PFSA?	Y	N	0.5	0.5	0.5	0.5	0.5
068187-47-3		PFSA?	Y	N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068140-20-5		Y	0.088	Fish 96-hour LC_{50} (mg/L)	
068140-21-6		Y	0.00104	Fish 96-hour LC_{50} (mg/L)	
068156-06-9		N	0.34	Fish 96-hour LC_{50} (mg/L)	
068187-47-3		Y	49040.289	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068140-20-5	68140205		Neutral Organics
068140-21-6	68140216		Neutral Organics
068156-06-9	68156069		Esters
068187-47-3	68187473		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068188-12-5	68188125	
	068259-14-3	68259143	
	068259-15-4	68259154	
	068298-11-3	68298113	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068188-12-5	FC(C(C(CCI)(F)F)(F)F)(F)F	F	3.43E+01	4.57E+03
068259-14-3	O=S(=O)(NC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	3.65E-01	4.87E+01
068259-15-4	O=S(=O)(NC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	4.97E-01	6.63E+01
068298-11-3	O=S(=O)(N(CCCN(CCO)(C)C)CCCS(=O)(=O)O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.93E-19	2.57E-17

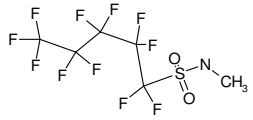
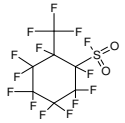
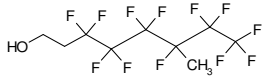
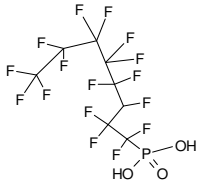
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068188-12-5	17.35	0.94	4.92	3.98	1228	3.089
068259-14-3	8.46	1.50	7.08	5.58	49600	4.695
068259-15-4	8.46	0.78	6.12	5.34	10240	4.010
068298-11-3	0.20	-18.27	2.27	20.54	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068188-12-5	Perfluorotelomer derivative? May degrade to perfluorobutanoic acid	neutral	N	N	
068259-14-3	Perfluoroheptanesulfonamide related. Phased out with PFOS related chemistry. Has been reported in Great lakes air.	neutral	Y	Y	
068259-15-4	Perfluorohexanesulfonamide related. Phased out with PFOS related chemistry. Has been reported in Great lakes air.	neutral	Y	Y	
068298-11-3	PFOS related sulfonamido alcohol. May be amenable to GC analysis.	acid	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068188-12-5		PFBA	Y	N	0.5				
068259-14-3		PFHpS	Y	N					
068259-15-4		PFHxS	Y	N					
068298-11-3		PFOS	Y	N		0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068188-12-5		N	1.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
068259-14-3		Y	4.42E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068259-15-4		Y	6.25E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068298-11-3		Y	588.479	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068188-12-5	68188125		Neutral Organics
068259-14-3	68259143		Esters + Peroxy Acids
068259-15-4	68259154		Neutral Organics
068298-11-3	68298113		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068298-13-5	68298135	
	068318-34-3	68318343	
	068391-08-2	68391082	
Top 10 fluorinated	068412-68-0	68412680	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068298-13-5	O=S(=O)(NC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	7.10E-01	9.47E+01
068318-34-3	O=S(=O)(C1(C(C(F)(F)C(C(C1(F)F)(F)F)(F)F)(C(F)(F)F)F)F)F	f	1.1	146.6546053
068391-08-2	OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	9.72E-02	1.30E+01
068412-68-0	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)P(=O)(O)O	F	5.21E-04	6.95E-02

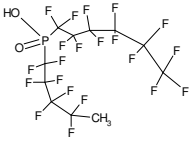
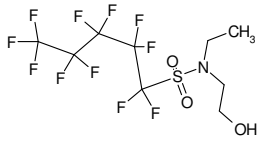
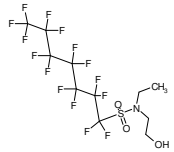
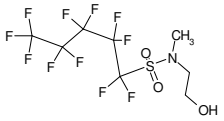
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068298-13-5	8.46	0.06	5.15	5.09	1847	3.266
068318-34-3		1.769791716	4.99	-0.174079105	1396	3.145
068391-08-2	2.56	2.23	7.53	5.30	12200	4.086
068412-68-0	38.20	-3.36	6.48	9.84	19510	4.290

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068298-13-5	Perfluoropentanesulfonamide related. Could be part of PFOS replacement chemistry - based on butane sulfonate	neutral	N	Y	
068318-34-3	Per F = P, cyclohexane metabolite, Maybe B	acid	N	N	
068391-08-2	Polyfluoro- telomer alcohol. Degradation products unknown. Likely analysable with other fluorotelomer alcohols	neutral	N	Y	
068412-68-0	Perfluoroalkyl (C6-C12) phosphonic acid . May be analysable as is by LC-MS. May degrade to PFNA or PFOA	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068298-13-5		PFPnS	Y	N					
068318-34-3		sulfonate	Y	N	0.5	0.5	0.5		
068391-08-2		PFCA?	Y	N	0.5	0.5			0.5
068412-68-0	Y	PFOA/PFNA	Y	N				0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068298-13-5		Y	0.15	Fish 96-hour LC_{50} (mg/L)	
068318-34-3			0.897	Fish 96-hour LC_{50} (mg/L)	
068391-08-2		Y	4.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068412-68-0		Y	3.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
068298-13-5	68298135		Neutral Organics
068318-34-3	68318343	MPV	Esters + Phenols + Salicylates
068391-08-2	68391082		Neutral Organics
068412-68-0	68412680		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068412-69-1	68412691	
	068555-72-6	68555726	
	068555-73-7	68555737	
	068555-74-8	68555748	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068412-69-1	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)P(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.11E-01	1.48E+01
068555-72-6	O=S(=O)(N(CCO)CC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	6.13E-05	8.17E-03
068555-73-7	O=S(=O)(N(CCO)CC)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	3.31E-05	4.41E-03
068555-74-8	O=S(=O)(N(CCO)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.08E-04	2.77E-02

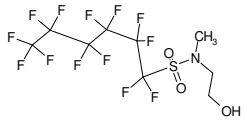
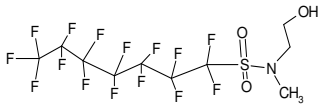
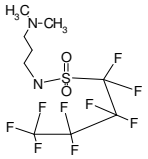
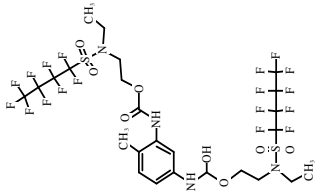
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
068412-69-1	76.40	2.90	9.87	6.97	8	0.882
068555-72-6	0.45	-3.79	4.88	8.67	1142	3.058
068555-73-7	0.45	-2.35	6.81	9.16	35110	4.545
068555-74-8	0.66	-3.92	4.39	8.31	478	2.679

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068412-69-1	Diperfluoroalkyl (C6-C12) phosphinic acid. May be analysable as is by LC-MS. May degrade to PFHxA or PFBA	neutral	N	N	
068555-72-6	1-Pentanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5, 5,5-undecafluoro-N-(2-hydroxyethyl)-. Could be part of PFOS replacement chemistry - based on butane sulfonate. Likely analysable by GC-MS with other fluoroalkylsulfonamides	neutral	Y	Y	
068555-73-7	Could be related to now phase out PFOS chemistry. Likely anlaysable by GC-MS with other fluoroalkylsulfonamides	neutral	Y	Y	
068555-74-8	Could be related to now phase out PFOS chemistry. Likely anlaysable by GC-MS with other fluoroalkylsulfonamides	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068412-69-1	Y	PFHxA/PFBA	Y	N				0.5	0.5
068555-72-6		PFPnS	Y	N			0.5		
068555-73-7		PFHxS/PFHpS	Y	N	0.5	0.5	0.5	0.5	
068555-74-8		PFPnS	Y	N	0.5	0.5	0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068412-69-1		Y	2.18E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
068555-72-6		Y	2.30E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068555-73-7		Y	1.08E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068555-74-8		Y	9.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068412-69-1	68412691		Neutral Organics
068555-72-6	68555726		Esters + Peroxy Acids
068555-73-7	68555737		Neutral Organics
068555-74-8	68555748		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068555-75-9	68555759	
	068555-76-0	68555760	
	068555-77-1	68555771	
	068608-13-9	68608139	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068555-75-9	O=S(=O)(N(CCO)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.51E-04	2.01E-02
068555-76-0	O=S(=O)(N(CCO)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	1.10E-04	1.47E-02
068555-77-1	O=S(=O)(NCCCN(C)C)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	2.47E-03	3.29E-01
068608-13-9	FC(C(C(C(S(N(CCOC(NC1=CC(=CC=C1C)NC(O)OCCN(S(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(=O)=O)CC)=O)CC)(=O)=O)(F)F)(F)F)(F)F)(F)F	F	1.82E-17	2.43E-15

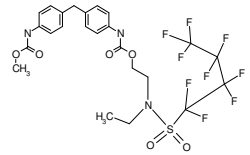
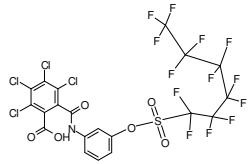
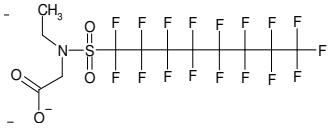
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068555-75-9	0.66	-3.20	5.36	8.56	2651	3.423
068555-76-0	0.66	-2.47	6.32	8.79	14700	4.167
068555-77-1	0.42	-4.72	4.37	9.09	465	2.668
068608-13-9	11.725 min	-14.00	8.17	22.17	363.1	2.560

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068555-75-9	Could be related to now phase out PFOS chemistry. Likely anlaysable by GC-MS with other fluoroalkylsulfonamides	neutral	Y	Y	
068555-76-0	Could be related to now phase out PFOS chemistry. Likely anlaysable by GC-MS with other fluoroalkylsulfonamides	neutral	Y	Y	
068555-77-1	N-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonamide. Could be part of PFOS replacement chemistry - based on butane sulfonate. Likely anlaysable by GC-MS with other fluoroalkylsulfonamides	neutral	Y	Y	
068608-13-9	Sulfonamides, C4-8-alkane, perfluoro, N-ethyl-N-(hydroxyethyl), reaction products with TDI. Likely analysable by GC-MS with other fluoroalkylsulfonamides.No structure. Similar to 68608-14-0 – SRC provided structure and SMILE	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068555-75-9		PFHxS/PFHpS	Y	N	0.5	0.5	0.5	0.5	
068555-76-0		PFHxS/PFHpS	Y	N	0.5	0.5	0.5	0.5	
068555-77-1		PFBS	Y	N			0.5	0.5	
068608-13-9		PFSA	Y	N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068555-75-9		Y	6.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068555-76-0		Y	4.32E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068555-77-1		N	2.52	Fish 96-hour LC_{50} (mg/L)	
068608-13-9		N	7.00E-02	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068555-75-9	68555759		Neutral Organics
068555-76-0	68555760		Aliphatic amine
068555-77-1	68555771		Neutral Organics
068608-13-9	68608139		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068608-14-0	68608140	
	068815-72-5	68815725	
	068867-62-9	68867629	No-Structure
	068891-96-3	68891963	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068608-14-0	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)N(CC)CCOC(=O)Nc1ccc(cc1)Cc2ccc(cc2)NC(=O)OCCN(CC)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	3.76E-16	5.01E-14
068815-72-5	[K]OC(=O)c2c(Cl)c(Cl)c(Cl)c(Cl)c2C(=O)Nc1cc(OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)ccc1	F	4.84E-21	6.45E-19
068867-62-9	No structure	F		
068891-96-3	CC(O[Cr]1(O[Cr](OC(=O1)CN(CC)S(=O)(=O)C(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(OC(C)C)(O)(Cl)Cl)(O)(Cl)Cl)C	F	1.57E-18	2.09E-16

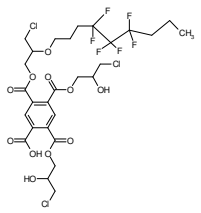
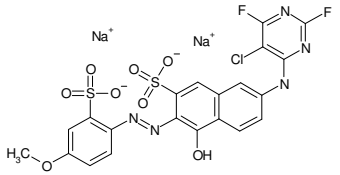
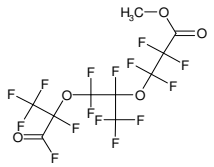
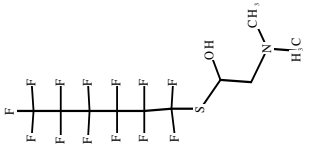
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068608-14-0	0.07	-10.40	12.63	23.03	3	0.500
068815-72-5	0.08	-13.39	7.10	20.49	3	0.500
068867-62-9						
068891-96-3	0.17	-9.03	7.69	16.72	7220	3.859

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068608-14-0	Sulfonamides, C4-8-alkane, perfluoro, N-ethyl-N-(hydroxyethyl), reaction products with 1,1'-methylenebis[4-isocyanatobenzene. Substituted perfluorosulfonamido compound. May be too polar for anlaysis by GC-MS.	neutral	N	Y?	
068815-72-5	1-Octanesulfonic acid,1,1,2,2, 3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, compounded with 2,2 -iminobis[ethanol] (1:1). Substituted perfluorosulfonamido compound. May be too polar for anlaysis by GC-MS. Amenable to LC-MS (ESI) with carboxylate group	acid	N	N	
068867-62-9	telomer with nonafluorobutyl. 2-[ethyl[(pentadecafluoroheptyl)sulfo nyl]amino]ethyl 2-methyl-2-propenoate,	acid	N	Y	
068891-96-3	Perfluorooctanesulfonamide - acetic acid derivative. May be analysable with other PFSAs by LC-MS	acid	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068608-14-0		PFBS	Y	N	0.5				
068815-72-5	Y	PFHxS and tetrachlorophthalate	Y	N	0.5	0.5	0.5	0.5	
068867-62-9		PFCA	Y	N					0.5
068891-96-3	Y	PFOS	Y	N	0.5	0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068608-14-0		N	5.05E-07	Fish 96-hour LC_{50} (mg/L)	
068815-72-5		Y	0.135	Fish 96-hour LC_{50} (mg/L)	
068867-62-9		Y	NA		
068891-96-3		Y	1.65E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068608-14-0	68608140		Phenols
068815-72-5	68815725		Neutral Organics
068867-62-9	68867629	MPV	Neutral Organics
068891-96-3	68891963		Esters + Esters (phosphate)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068954-01-8	68954018	
	068959-17-1	68959171	
	069116-73-0	69116730	
	070983-60-7	70983607	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068954-01-8	OC(=O)c1cc(c(cc1C(=O)OCC(CCl)O)C(=O)OCC(CCl)O)C(=O)OCC(CCl)OCCCCC(C(C(CCC)(F)F)(F)F)(F)F	F	4.88E-21	6.51E-19
068959-17-1	c1cc(OC)cc(S(=O)(=O)O[Na])c1N=Nc2c(O)c3ccc(cc3cc2S(=O)(=O)O[Na])Nc4nc(F)nc(F)c4Cl	f	3.13E-27	4.17299E-25
069116-73-0	O=C(OC)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)(C(=O)F)C(F)(F)F	f	0.0205	2.733108553
070983-60-7	C(C(C(C(C(C(SC(CN(C)C)O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	5.07E-02	6.76E+00

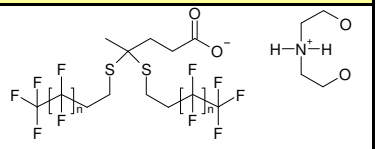
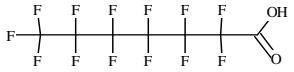
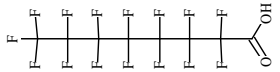
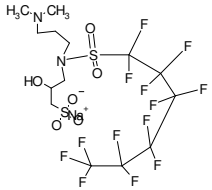
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068954-01-8	0.42	-18.58	6.59	25.17	56	1.750
068959-17-1	2.471402903	-29.07260043	-1.06	24.61831304	3.162	0.500
069116-73-0	1179.784825	-2.158121855	3.61	2.373834466	120.9	2.082
070983-60-7	1.6 h	-4.61	4.87	9.48	1129.8	3.053

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068954-01-8	1,2,4,5-Benzenetetracarboxylic acid, mixed 3-chloro-2-hydroxypropyl and γ-ω-perfluoro-C8-14-alkyl esters. Very polar. May be amenable to LC-MS	neutral	N	N	
068959-17-1	Di F, Cl pyrimidine = P metabolite?	acid	N	N	
069116-73-0	Maybe P (per F, but ester and acid fluroide, not B	acid	N	Y?	
070983-60-7	3-(1,1,2,2-Tetrahydroperfluoro(C6-C20)alkylthio)-2-hydroxypropyl)trimethylammonium chloride. May have fluorotelomer chain which could degrade to PFCAs	amine	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068954-01-8	Y?			N	0.5	0.5	0.5		
068959-17-1	Y	?		N	0.5	0.5	0.5		
069116-73-0		PFCA	Y?	N	0.5		0.5	0.5	0.5
070983-60-7		PFCA	Y	N		0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068954-01-8		Y	0.318	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068959-17-1			66.759	Fish 96-hour LC_{50} (mg/L)	
069116-73-0			4.968	Fish 96-hour LC_{50} (mg/L)	
070983-60-7		Y	1.76E+00	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068954-01-8	68954018		Esters + Esters (phosphate)
068959-17-1	68959171	MPV	Neutral Organics
069116-73-0	69116730	MPV	Neutral Organics
070983-60-7	70983607		Esters + Esters (phosphate)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	071608-61-2	71608612	
	072623-77-9	72623779	
	072968-38-8	72968388	
	073772-32-4	73772324	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
071608-61-2	FC(C(C(C(C(C(CCSC(SCCC(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C)CCN(CCO)CCO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	3.60E-10	4.80E-08
072623-77-9	FC(C(C(C(C(C(C(O)=O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	1.12E+00	1.49E+02
072968-38-8	C(C(C(C(C(C(C(C(O)=O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	F	5.25E-01	7.00E+01
073772-32-4	O=S(CC(O)CN(CCCN(C)C)S(=O)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)=O)([O-])=O.[Na+]	F	3.17E-19	4.23E-17

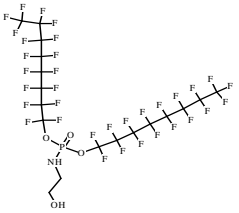
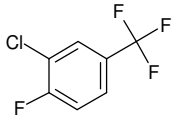
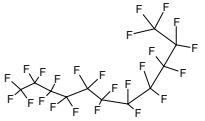
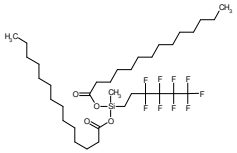
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
071608-61-2	2.03	-2.54	13.99	16.53	3.2	0.500
072623-77-9	20.56 days	-0.15	5.33	5.48	5.6	0.750
072968-38-8	20.56 days	0.57	6.30	5.73	56.2	1.750
073772-32-4	0.22	-13.90	0.60	14.50	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
071608-61-2	Pentanoic acid, 4,4-bis[(gamma-omega-perfluoro-C8-20-alkyl)thio] derivatives. May degrade to PFCAs	amine	N	N	
072623-77-9	C6-18, perfluoro, ammonium salts. May refer to mixture of PFCAs. No structure (perfluorocarboxylates) – SRC provided SMILE	polymer	N	Y	
072968-38-8	Fatty acids, C7-13, perfluoro, ammonium salts. May refer to mixture of PFCAs. No structure (perfluorocarboxylates) – SRC provided SMILE	acid	N	Y	
073772-32-4	Perfluorosulfonamido alcohol. Yields PHHxS on degradation	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
071608-61-2		PFCA	Y	N	0.5	0.5	0.5	0.5	0.5
072623-77-9		PFCA	Y	N					0.5
072968-38-8		PFCA	Y	N		0.5		0.5	
073772-32-4		PFHxS	Y	N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
071608-61-2		Y	5.36E-06	Fish 96-hour LC_{50} (mg/L)	
072623-77-9		Y	5.40E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
072968-38-8		Y	4.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
073772-32-4		Y	1.40E+03	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
071608-61-2	71608612		Esters + Esters (phosphate)
072623-77-9	72623779		Neutral Organics
072968-38-8	72968388		Neutral Organics
073772-32-4	73772324		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	074499-44-8	74499448	
	078068-85-6	78068856	
	086508-42-1	86508421	
	094094-26-5	94094265	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
074499-44-8	C(C(C(C(C(C(C(OP(OC(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(=O)NCCO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(F)(F)F)(F)F	F	6.03E-05	8.04E-03
078068-85-6	FC(c1ccc(c(c1)Cl)F)(F)F	f	6.06	807.9335526
086508-42-1	FC(C(C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)F	F	1.79E+00	2.39E+02
094094-26-5	CCCCCCCCCCCCCC(=O)O[Si](CCC(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(C)C	F	2.66E-05	3.55E-03

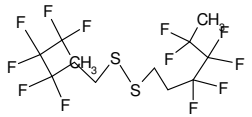
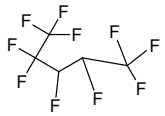
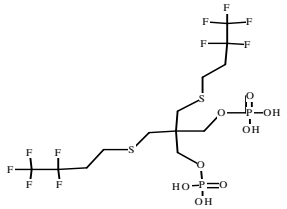
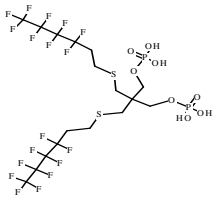
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
074499-44-8	8.646 h	0.72	13.46	12.74	3.16	1
078068-85-6	895.4973419	0.218884247	3.8	0.186828364	168.5	2.227
086508-42-1		9.48	10.85	1.37	3	0.500
094094-26-5	0.62	2.91	12.34	9.43	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
074499-44-8	Phosphoric acid, perfluoro-C8-16-alkyl esters, compounds with diethanolamine. Could yield C8-C16 PFCAs on degradation. Google search indicates it is a DEA-C8Cr8 perfluoroalkylethyl phosphate. No structure (similar to 68412-68-0) – SRC provided SMILE	neutral	N	N	
078068-85-6	P but probably not B	neutral	N	Y	
086508-42-1	CAS # refers to class of inert perfluoroalkanes formed by electrochemical fluorination. Highly volatile. GW potential. Could be analysable by GC modified for gas analysis	neutral	N	Y	
094094-26-5	Tetradecanoic acid, methyl(3,3,4,4,5,5,6,6,6-nonafluorohexyl)silylene ester. Much lower VP than other PFCs or siloxanes due to hydrocarbon side chains. Amenable to GC-MS analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
074499-44-8		PFCA	Y	N					0.5
078068-85-6				N	0.5	0.5		0.5	
086508-42-1				N	10	50	10	50	10
094094-26-5				N		0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
074499-44-8		Y	1.37E--7	Fish 96-hour LC_{50} (mg/L)	
078068-85-6			3.982	Fish 96-hour LC_{50} (mg/L)	Marginal
086508-42-1		N	1.09E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
094094-26-5		N	5.57E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
074499-44-8	74499448		Neutral Organics
078068-85-6	78068856	MPV	Neutral Organics
086508-42-1	86508421		Neutral Organics
094094-26-5	94094265		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	118400-71-8	118400718	
	138495-42-8	138495428	
	148240-85-1	148240851	
	148240-87-3	148240873	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
118400-71-8	CC(C(C(CCSSCCC(C(C(C)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	9.46E-02	1.26E+01
138495-42-8	C(F)(F)(F)C(F)C(F)C(F)(F)C(F)(F)F	F	1.09E+03	1.45E+05
148240-85-1	FC(C(CCSCC(CSCCC(C(F)(F)F)(F)F)(COP(=O)(O)O)COP(=O)(O)O)(F)F)(F)F	F	2.06E-11	2.75E-09
148240-87-3	C(CSCC(CSCCC(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(COP(=O)(O)O)COP(=O)(O)O)C(C(C(C(F)(F)F)(F)F)(F)F)(F)F	F	2.06E-11	2.75E-09

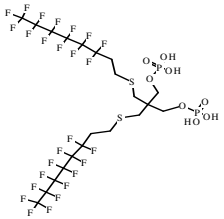
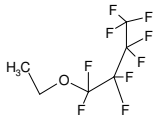
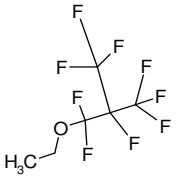
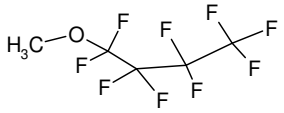
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
118400-71-8	0.04	2.51	9.63	7.12	16	1.201
138495-42-8	3136.65	2.96	3.84	0.88	180	2.255
148240-85-1	1.476 h	-20.209	4.49	24.70	576.8	2.761
148240-87-3	1.48	-17.33	8.36	25.69	887.2	2.948

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
118400-71-8	Disulfides, bis(γ-ω-perfluoro-C6-20-alkyl). Use unknown. Likely to be analysable by GC-MS with other polyfluoroalkyl alcohols and amidoalcohols	neutral	N	Y	
138495-42-8	2H,3H-Decafluoropentane. Highly volatile. GW potential. Could be analysable by GC modified for gas analysis	neutral	N	Y	
148240-85-1	1,3-Propanediol, 2,2-bis[[(gamma-omega-perfluoro-C4-10-alkyl)thio]methyl] derivatives, phosphates. Could yield C4-C10 PFCAs on degradation. No structure (similar to 68412-68-0) – SRC provided structure and SMILE	neutral	N	N	
148240-87-3	1,3-Propanediol, 2,2-bis[[(gamma-omega-perfluoro-C6-12-alkyl)thio]methyl] derivatives, phosphates, ammonium salts. Could yield C6-C12 PFCAs on degradation. No structure (similar to 68412-68-0) – SRC provided SMILE	neutral	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
118400-71-8				N		0.5		0.5	0.5
138495-42-8				N				0.5	1
148240-85-1		PFCA	Y	N				0.5	
148240-87-3		PFCA	Y	N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
118400-71-8		N	2.79E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	
138495-42-8		N	2.70E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
148240-85-1		Y	1.02E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
148240-87-3		Y	1.97E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
118400-71-8	118400718		Neutral Organics
138495-42-8	138495428		Neutral Organics
148240-85-1	148240851		Neutral Organics
148240-87-3	148240873		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	148240-89-5	148240895	
	163702-05-4	163702054	
	163702-06-5	163702065	
	163702-07-6	163702076	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
148240-89-5	C(CSCC(CSCCC(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(COP(=O)(O)O)COP(=O)(O)O)C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	F	2.06E-11	2.75E-09
163702-05-4	FC(F)(F)C(F)(F)C(F)(F)C(F)(OCC)F	F	3.50E+02	4.67E+04
163702-06-5	FC(F)(F)C(F)(C(F)(OCC)F)C(F)(F)F	f	350	46662.82895
163702-07-6	COC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	F	9.05E+02	1.21E+05

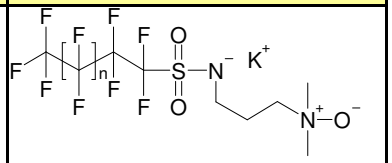
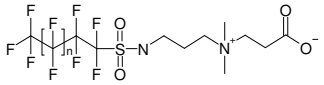
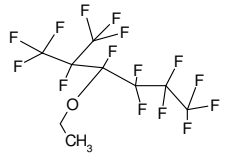
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
148240-89-5	1.48	-14.45	12.22	26.67		
163702-05-4	16.14	0.73	4.42	3.69	507	2.705
163702-06-5	193.6641355	1.72870052	3.72	-1.402987908	145.3	2.162
163702-07-6	393.23	0.61	3.93	3.33	212	2.327

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
148240-89-5	1,3-Propanediol, 2,2-bis[[(gamma-omega-perfluoro-C10-20-alkyl)thio]methyl] derivatives, phosphates. Could yield C10-C20 PFCAs on degradation. No structure (similar to 68412-68-0) – SRC provided SMILE	neutral	N	N	
163702-05-4	Fluoroether. Cleaning solvent and blowing agents. GW activity. Could be analysable by GC modified for gas analysis	neutral	N	Y	
163702-06-5	Per F = P, GWP	neutral	N	Y	
163702-07-6	Fluoroether. Cleaning solvent and blowing agents. GW activity. Could be analysable by GC modified for gas analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
148240-89-5		PFCA	Y	N				0.5	
163702-05-4				N				0.5	0.5
163702-06-5				N				0.5	0.5
163702-07-6				N				1	1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
148240-89-5		Y	3.66E-11	Mysid Shrimp 96-hour LC_{50} (mg/L)	
163702-05-4		Y	5.30E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
163702-06-5		N	0.4	Mysid Shrimp 96-hour LC_{50} (mg/L)	
163702-07-6		Y	2.07E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
148240-89-5	148240895		Neutral Organics
163702-05-4	163702054		Neutral Organics
163702-06-5	163702065	MPV	Silanes (alkoxy)
163702-07-6	163702076		Silanes (alkoxy)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	179005-06-2	179005062	
	192662-29-6	192662296	
	212335-64-3	212335643	No-Structure
	297730-93-9	297730939	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
179005-06-2	FC(C(C(C(S(NCCCN(O)(C)C)(=O)=O)(F)F)(F)F)(F)F)(F)F No structure similar to **68608-14-0 –** SRC provided structure and SMILE	F	5.44E-12	7.25E-10
192662-29-6	FC(C(C(C(S(NCCCN(C)(C)CCC(O)=O)(=O)=O)(F)F)(F)F)(F)F)(F)F No structure similar to 68608-14-0 – SRC provided structure and SMILE	F	1.49E-11	1.99E-09
212335-64-3		f		
297730-93-9	CCOC(F)(C(F)(F)C(F)(F)C(F)(F)F)C(F)(C(F)(F)F)C(F)(F)F	F	2.20E+01	2.96E+03

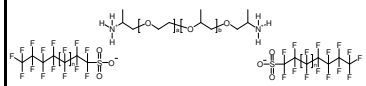
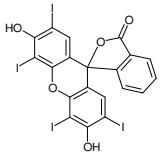
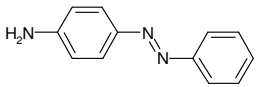
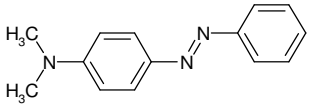
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
179005-06-2	5.07 h	-13.70	1.31	15.01	20.42	1
192662-29-6	3.43 h	-15.67	1.15	16.82	14.13	1
212335-64-3						
297730-93-9	16.38	2.89	6.07		9345	3.970

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
179005-06-2	Sulfonamides, C4-8-alkane, perfluoro, N-[3-(dimethyloxidoamino)propyl], potassium salts. Related to PFOS or replacement perfluorobutane sulfonate chemistry	amine	N	N	
192662-29-6	Sulphonamides, C4-8-alkane, perfluoro, N-[3-(dimethylamino)propyl], reaction products with acrylic acid. Related to PFOS or replacement perfluorobutane sulfonate chemistry	acid	N	N	
212335-64-3	Per F = P, C4 metabolites; 2-Propenoic acid, reaction products with N-[3-(dimethylamino)propyl]-. 1,1,2,2,3,3,4,4,4-nonafluoro-1-butanesulfonamide	acid	N	Y	
297730-93-9	Fluoroether. 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-trifluoromethyl-hexane. Cleaning solvent and blowing agents. GW potential. Could be analysable by GC modified for gas analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
179005-06-2		PFSA?	Y	N				0.5	
192662-29-6		PFSA?	Y	N					0.5
212335-64-3		PFSA?	Y	N				1	0.5
297730-93-9				N					0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
179005-06-2		N	3.06E+02	Fish 96-hour LC_{50} (mg/L)	
192662-29-6		Y	1.13E+04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
212335-64-3		Y	NA	NA	
297730-93-9		N	7.24E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
179005-06-2	179005062		Neutral Organics
192662-29-6	192662296		Phenols
212335-64-3	212335643	MPV	Neutral Organics
297730-93-9	297730939		Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	306974-45-8	306974458	
	015905-32-5	15905325	
	000060-09-3	60093	
	000060-11-7	60117	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
306974-45-8	FC(C(C(C(S(NC(COCCOC(COCC(NS(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(=O)=O)C)C)C)(=O)=O)(F)F)(F)F)(F)F)(F)F No structure similar to **68608-14-0 –** SRC provided structure and SMILE	F	1.81E-09	2.41E-07
015905-32-5	O=C(OC(c(c(Oc1c(c(O)c(c2)I)I)c(c(O)c3I)I)c3)(c12)c4cccc5)c45	I	3.93E-20	5.24E-18
000060-09-3	N(=Nc(cccc1)c1)c(ccc(N)c2)c2	non-halo	0.00000526	0.000701276
000060-11-7	N(=Nc(cccc1)c1)c(ccc(N(C)C)c2)c2	non-halo	0.0000372	0.004959592

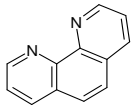
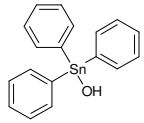
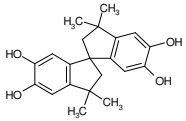
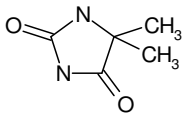
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
306974-45-8	0.73	-6.74	8.46	15.20	647.1	2.811
015905-32-5	1.82	-16.98	8.02	25.00	1031	3.013
000060-09-3	2.955531361	-6.672567432	3.19	6.468280044	10	1.000
000060-11-7	0.85655327	-5.019354919	4.29	5.91506753	10	1.000

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
306974-45-8	Sulphonic acids, C6-8-alkane, perfluoro, compounds with polyethylene-polypropylene glycol bis(2-aminopropyl) ether. Related to PFOS or replacement perfluorobutane sulfonate chemistry	neutral	N	N	
015905-32-5	Pigment and dye. Erythrosine acid. Highly polar with 2 phenolic groups. May be amenable to LC-MS analysis	phenol	N	N	
000060-09-3		amine	N	Y?	
000060-11-7		neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
306974-45-8		PFSA?	Y	N					0.5
015905-32-5	Y?			N	0.5	0.5			
000060-09-3				N	0.5	1	0.5	0.5	0.5
000060-11-7				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
306974-45-8		Y	1.40E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
015905-32-5		Y	0.002	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000060-09-3		Y	7.827	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000060-11-7		Y	0.066	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
306974-45-8	306974458		Phenols (dinitro)
015905-32-5	15905325		Neutral Organics
000060-09-3	60093	airbreather	Neutral Organics
000060-11-7	60117	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000066-71-7	66717	
	000076-87-9	76879	
	000077-08-7	77087	
	000077-71-4	77714	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000066-71-7	n(c(c(ccc1cccn2)cc3)c12)c3	non-halo	0.0000239	0.003186405
000076-87-9	O[Sn](c1ccccc1)(c2ccccc2)c3ccccc3	Non-halo	1.14E-08	1.52E-06
000077-08-7	Oc(c(O)cc(c1C(c(c(cc(O)c2O)C3(C)C)c2)(C4)C3)C4(C)C)c1	non-halo	8.38E-12	1.11724E-09
000077-71-4	O=C(NC(C1=O)(C)C)N1	Non-halo	1.36E-06	1.81E-04

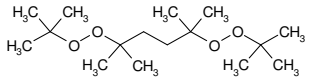
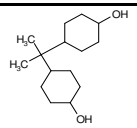
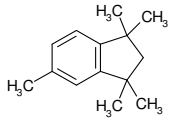
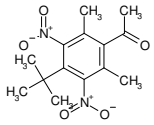
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000066-71-7	64.1802945	-8.444088104	2.29	7.339800715	17.09	1.233
000076-87-9	1.79	-5.73	3.47	9.20	2619	3.418
000077-08-7	1.032517466	-17.52584325	5.29	19.42155586	2381	3.377
000077-71-4	3.49	-6.95	-0.27	6.68	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000066-71-7		neutral	N	Y	
000076-87-9	May be analysable with similar methodology as trialkyl tins	phenol	N	N	Y
000077-08-7	Large B if it doesn't metabolize. May be P but has two catachol rings that may be biodegraded	phenol	N	N	Y
000077-71-4	5,5-Dimethylhydrantoin. Not bioaccumulative but possibly persistent to due dimethyl substitution	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000066-71-7				N	0.5	0.5	0.5	0.5	0.5
000076-87-9	Y?			N	0.5	10			
000077-08-7	Y?			N	0.5				
000077-71-4				N	10	10	50	50	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000066-71-7		Y	16.72	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000076-87-9		Y	9.60E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000077-08-7		Y	0.47	Fish 96-hour LC_{50} (mg/L)	
000077-71-4		Y	5.35E+03	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000066-71-7	66717	airbreather	Neutral Organics
000076-87-9	76879		Neutral Organics
000077-08-7	77087	MPV	Neutral Organics
000077-71-4	77714		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000078-63-7	78637	
	000080-04-6	80046	
	000081-03-8	81038	
	000081-14-1	81141	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000078-63-7	O(OC(C)(C)C)C(CCC(OOC(C)(C)C)(C)C)(C)C	Non-halo	4.22E-03	5.63E-01
000080-04-6	OC(CCC(C(C(CCC(O)C1)C1)(C)C)C2)C2	non-halo	0.000000507	6.75944E-05
000081-03-8	c(c(ccc1C)C(C2)(C)C)(c1)C2(C)C	non-halo	0.0214	2.853098684
000081-14-1	O=C(c(c(c(N(=O)(=O))c(c1N(=O)(=O))C(C)(C)C)C)c1C)C	non-halo	0.000000315	4.19965E-05

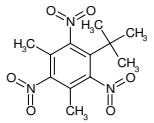
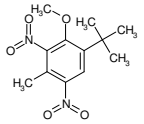
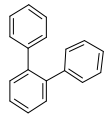
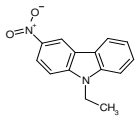
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000078-63-7	2.38	-0.98	6.55	7.53	22240	4.347
000080-04-6	3.234544173	-4.384249402	4.55	5.539962014	641.5	2.807
000081-03-8	8.465315119	-0.267996845	5.76	2.633709456	5395	3.732
000081-14-1	99.29573454	-7.707329539	4.31	8.62304215	60.41	1.781

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000078-63-7	2,5-Dimethyl-2,5-Bis(Tert-Butyl Peroxy)Hexane. Polymerization initiator	neutral	N	Y	
000080-04-6		neutral	N	N	Y
000081-03-8	No prod lately. Might be polycyclic musk. High branching (P) and high Kow (B)	neutral	Y	Y	
000081-14-1	Nitro musk - probably detected already	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000078-63-7				N	1	10	10	10	10
000080-04-6				N	0.5	0.5	0.5	0.5	0.5
000081-03-8				Y	0.5				
000081-14-1				Y	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000078-63-7		Y	0.031	Fish 96-hour LC_{50} (mg/L)	
000080-04-6		Y	0.169	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000081-03-8		Y	0.005	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000081-14-1		Y	0.279	Fish 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000078-63-7	78637		Vinyl/Allyl Ketones
000080-04-6	80046	airbreather	Vinyl/Allyl Ethers
000081-03-8	81038	MPV	Neutral Organics
000081-14-1	81141	MPV	Acrylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000081-15-2	81152	
	000083-66-9	83669	
	000084-15-1	84151	
	000086-20-4	86204	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000081-15-2	N(=O)(=O)c(c(c(N(=O)(=O))c(c1N(=O)(=O))C(C)(C)C)C)c1C	non-halo	0.000000635	8.46597E-05
000083-66-9	N(=O)(=O)c(c(c(N(=O)(=O))c(OC)c1C(C)(C)C)C)c1	non-halo	0.0000131	0.001746523
000084-15-1	c(c(c(cccc1)c1)ccc2)(c(cccc3)c3)c2	non-halo	0.000181	0.024131349
000086-20-4	O=N(=O)c(ccc(N(c(c1ccc2)c2)CC)c13)c3	non-halo	0.00000137	0.000182652

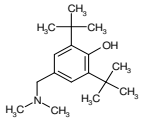
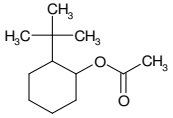
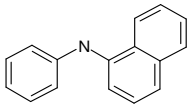
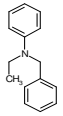
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000081-15-2	154.4670682	-7.371537437	4.45	8.427250048	532.9	2.727
000083-66-9	85.44726404	-6.239351663	4.17	7.015064275	322	2.508
000084-15-1	13.96041692	-2.886143656	5.52	5.011856268	3558	3.551
000086-20-4	1.124039393	-5.908563833	4.15	6.664276445	311.5	2.493

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000081-15-2	Nitro musk - probably detected already. Explosive?	neutral	Y	Y	
000083-66-9	Nitro musk. ' Nitro musk. 8 monitoring refs in DL	neutral	Y	Y	
000084-15-1	No recent production	neutral	N	Y	
000086-20-4		neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000081-15-2				Y	1	0.5	0.5	0.5	0.5
000083-66-9				Y	0.5				
000084-15-1				N			0.5		
000086-20-4				N	0.5		0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000081-15-2		Y	0.23	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000083-66-9		Y	0.317	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000084-15-1		Y	0.011	Mysid Shrimp 96-hour LC50 (mg/L)	
000086-20-4		Y	0.515	Mysid Shrimp 96-hour LC50 (mg/L)	moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000081-15-2	81152	MPV	Esters + Phenols
000083-66-9	83669	MPV	Esters + Phenols
000084-15-1	84151	MPV	Vinyl/Allyl Ketones + Vinyl/Allyl Halides + Vinyl/Allyl Ethers
000086-20-4	86204	airbreather	Benzyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000088-27-7	88277	
	000088-41-5	88415	
	000090-30-2	90302	
	000092-59-1	92591	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000088-27-7	Oc(c(cc(c1)CN(C)C)C(C)(C)C)c1C(C)(C)C	non-halo	0.0000101	0.001346556
000088-41-5	O=C(OC(C(C(C)(C)C)CCC1)C1)C	Non-halo	6.85E-02	9.13E+00
000090-30-2	N(c(c(c(ccc1)cc2)c1)c2)c(cccc3)c3	non-halo	0.0000289	0.003853016
000092-59-1	N(c(cccc1)c1)(Cc(cccc2)c2)CC	non-halo	0.00299	0.398633882

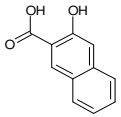
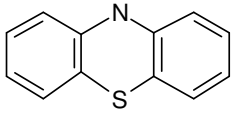
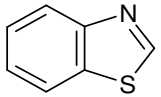
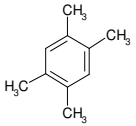
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000088-27-7	1.357606007	-7.076816915	4.24	7.922529527	129.2	2.111
000088-41-5	0.74	-1.39	4.42	5.81	507	2.705
000090-30-2	0.370390473	-5.375733551	4.47	6.451446163	342	2.534
000092-59-1	0.759802068	-3.425728095	4.07	4.101440706	271.3	2.433

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000088-27-7		neutral	N	N	Y
000088-41-5	ester that will hydrolyze to 2-t-butylcyclohexanol Kow 4.42 but less for alcohol	neutral	N	Y	
000090-30-2		neutral	N	Y	
000092-59-1	tertiary amine = P?	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000088-27-7				N		0.5	0.5	0.5	0.5
000088-41-5		t-butylphenol	Y	N	0.5	0.5	1	10	10
000090-30-2				N	10	10	10	10	10
000092-59-1				N	10	1	10	10	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000088-27-7		Y	0.907	Fish 96-hour LC_{50} (mg/L)	
000088-41-5		Y	0.448	Mysid Shrimp 96-hour LC50 (mg/L)	
000090-30-2		Y	0.196	Mysid Shrimp 96-hour LC50 (mg/L)	
000092-59-1		N	0.56	Mysid Shrimp 96-hour LC50 (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000088-27-7	88277	airbreather	Neutral Organics
000088-41-5	88415		Neutral Organics
000090-30-2	90302	airbreather	Imides
000092-59-1	92591	airbreather	Imides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000092-70-6	92706	
	000092-84-2	92842	
	000095-16-9	95169	
	000095-93-2	95932	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000092-70-6	O=C(O)c(c(O)cc(c1ccc2)c2)c1	non-halo	6.23E-08	8.30598E-06
000092-84-2	N(c(c(Sc1cccc2)ccc3)c3)c12	Non-halo	8.32E-07	1.11E-04
000095-16-9	c1ccc2ncsc2c1	non-halo	0.0742	9.892519737
000095-93-2	c(c(cc(c1C)C)C)(c1)C	Non-halo	1.18E-01	1.57E+01

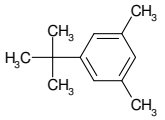
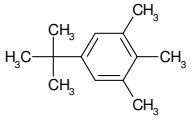
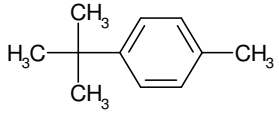
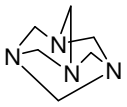
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000092-70-6	5.302169352	-7.245555976	3.42	7.271268587	3.162	0.500
000092-84-2	0.06	-5.94	3.82	9.76	313	2.496
000095-16-9	18.337227	-4.815699174	2.17	3.591411785	7.042	0.848
000095-93-2	0.52	-0.49	4.18	4.67	240	2.380

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000092-70-6	DSL = P experimental?	acid	N	N	Y
000092-84-2	N,S heterocyclo Kow 4.15 looks persistent	neutral	N	Y	
000095-16-9	DSL P experimental, look at all benzothiazoles	neutral	N	Y	
000095-93-2	Solvent use? Analysable with other hydrocarbons/substituted benzenes by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000092-70-6				N	10	10	50	50	50
000092-84-2				N	0.5		10	10	10
000095-16-9				N	1	0.5	1	10	10
000095-93-2				N	10	50	10	1	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000092-70-6		Y	25.571	Fish 96-hour LC_{50} (mg/L)	Low
000092-84-2		N	8.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000095-16-9		Y	65.398	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000095-93-2		Y	9.10E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000092-70-6	92706	airbreather	Neutral Organics
000092-84-2	92842		Neutral Organics
000095-16-9	95169	airbreather	Neutral Organics
000095-93-2	95932		Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000098-19-1	98191	
	000098-23-7	98237	
	000098-51-1	98511	
	000100-97-0	100970	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000098-19-1	c(cc(cc1C)C(C)(C)C)(c1)C	non-halo	0.254	33.86388158
000098-23-7	c(cc(c(c1C)C)C)(c1)C(C)(C)C	non-halo	0.0798	10.639125
000098-51-1	c(ccc(c1)C)(c1)C(C)(C)C	Non-halo	5.92E-01	7.89E+01
000100-97-0	N(CN(CN1CN23)C3)(C1)C2	Non-halo	9.10E-02	1.21E+01

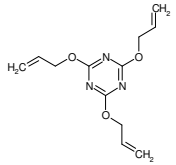
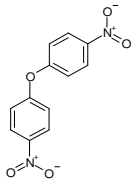
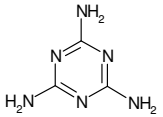
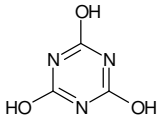
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000098-19-1	4.271510163	-0.160684071	5	1.766396683	1405	3.148
000098-23-7	3.488179864	-0.116729169	5.54	2.262441781	3708	3.569
000098-51-1	1.59	-0.20	4.45	4.65	1909	3.281
000100-97-0	0.02	0.82	-4.15	-4.97	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000098-19-1	Trimethyl are P this should be more, BCF 1000	neutral	N	Y	
000098-23-7	P&B	neutral	N	Y	
000098-51-1	Analysable with other hydrocarbons/substituted benzenes by GC-MS	neutral	Y	Y	
000100-97-0	Methenamine. looks very persistent and production is 50-100M all 5 years. HSDB - 56% AS A CURING AGENT FOR PHENOLIC RESINS; 37% AS A CHEM INT FOR THE EXPLOSIVE, CYCLONITE; & 7% IN MISC APPLICATIONS (1974). Has been measured for occupational exposure	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000098-19-1				N		0.5	0.5	0.5	
000098-23-7				N	0.5				
000098-51-1				Y	10		10	10	0.5
000100-97-0				Y	100	100	100	100	100

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000098-19-1		Y	0.034	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000098-23-7		Y	0.008	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000098-51-1		Y	3.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000100-97-0		Y	1.24E+05	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000098-19-1	98191	MPV	Benzyl Halides
000098-23-7	98237	MPV	Imides
000098-51-1	98511		Imides
000100-97-0	100970		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000101-37-1	101371	
	000101-63-3	101633	
	000108-78-1	108781	
	000108-80-5	108805	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000101-37-1	O(c(nc(OCC=C)nc1OCC=C)n1)CC=C	Non-halo	2.26E-05	3.01E-03
000101-63-3	O=N(=O)c(ccc(Oc(ccc(N(=O)=O)c1)c1)c2)c2	non-halo	0.000000738	9.83919E-05
000108-78-1	n(c(nc(n1)N)N)c1N	Non-halo	8.93E-08	1.19E-05
000108-80-5	N1C(=O)NC(=O)NC1=O	Non-halo	5.26E-09	7.01E-07

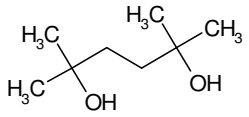
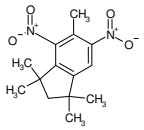
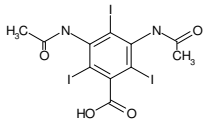
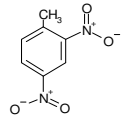
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000101-37-1	0.32	-4.76	5.27	10.03	3	0.482
000101-63-3	137.7717792	-7.126119686	3.68	7.411832298	137.2	2.137
000108-78-1	16.22	-11.11	-0.38	10.73	3	0.500
000108-80-5	3.57	-12.45	1.95	14.40	6	0.803

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000101-37-1	Triallyl cyanurate . May be analysable by GC-MS simil to triazine herbicides	neutral	N	Y	
000101-63-3	P - two Nitro, one ether	neutral	N	Y	
000108-78-1	Melamine. Many uses. Methodology available for occupational exposure and food contamination	amine	N	Y	
000108-80-5	Isocyanuric acid. Methodology available for occupational exposure and food contamination	phenol	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000101-37-1				N	0.5	1	1	10	0.5
000101-63-3				N	10	10			
000108-78-1				N	500	500	500	500	500
000108-80-5				N	50	100	500	500	500

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000101-37-1		Y	1.56E-01	Fish 96-hour LC_{50} (mg/L)	
000101-63-3		Y	1.98	Mysid Shrimp 96-hour LC_{50} (mg/L)	high
000108-78-1		Y	1863.183	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000108-80-5		Y	7.67E+01	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000101-37-1	101371		polymer
000101-63-3	101633	airbreather	Neutral Organics
000108-78-1	108781		Vinyl/Allyl Ketones
000108-80-5	108805		Halo alcohols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000110-03-2	110032	
	000116-66-5	116665	
	000117-96-4	117964	
	000121-14-2	121142	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000110-03-2	OC(CCC(O)(C)C)(C)C	Non-halo	4.33E-03	5.77E-01
000116-66-5	N(=O)(=O)c(c(c(N(=O)(=O))c(c1C(C2)(C)C)C2(C)C)C)c1	Non-halo	1.71E-06	2.28E-04
000117-96-4	CC(=O)Nc1c(I)c(NC(=O)(C))c(I)c(C(=O)(O))c1I	Non-halo	3.57E-15	4.76E-13
000121-14-2	N(=O)(=O)c(ccc(c1N(=O)(=O))C)c1	non-halo	0.000719	0.095858783

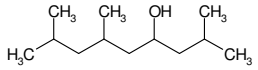
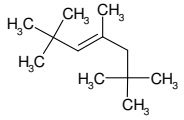
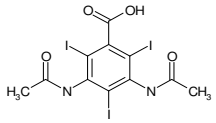
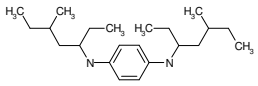
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000110-03-2	0.97	-4.53	1.52	6.05	3	0.474
000116-66-5	6.09	-5.08	5.39	10.47	2826	3.451
000117-96-4	7.12	-15.94	1.37	17.31	3	0.500
000121-14-2	595.6131455	-5.421959789	2.18	4.207672401	6.677	0.825

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000110-03-2	2,5-Dimethyl-2,5-hexanediol . di-tertiary alcohol - probably somewhat persistent in ground water.	neutral	N	Y	
000116-66-5	Musk Moskene. See other musks	neutral	Y	Y	
000117-96-4	Diatrizoic acid. Radio contrast chemical? May be analysable by GC-MS after derivatization	acid	N	N	Y
000121-14-2	P two Nitro	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000110-03-2				N	1	10	10	10	10
000116-66-5				Y	0.5	0.5	0.5	0.5	
000117-96-4				N					
000121-14-2				N	500	500	1000	1	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000110-03-2		Y	413.13	mysid Shrimp 96-hour LC50 (mg/L)	
000116-66-5		Y	0.053	Fish 96-hour LC_{50} (mg/L)	
000117-96-4		N	1628.264	Fish 96-hour LC_{50} (mg/L)	Low
000121-14-2		Y	4.138	Fish 96-hour LC_{50} (mg/L)	High-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000110-03-2	110032		Acrylamides
000116-66-5	116665		Phenols
000117-96-4	117964		Benzyl Halides
000121-14-2	121142	airbreather	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000123-17-1	123171	
	000123-48-8	123488	
	000131-49-7	131497	
	000139-60-6	139606	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000123-17-1	OC(CC(CC(C)C)C)CC(C)C	non-halo	0.0158	2.106493421
000123-48-8	C(=CC(C)(C)C)(CC(C)(C)C)C	non-halo	1.32	175.9855263
000131-49-7	CC(=O)Nc1c(I)c(C(=O)O)c(I)c(NC(=O)C)c1I	Non-halo	3.57E-15	4.76E-13
000139-60-6	N(c(ccc(NC(CC)CC(CC)C)c1)c1)C(CC)CC(CC)C	non-halo	0.00000145	0.000193317

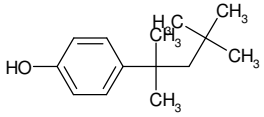
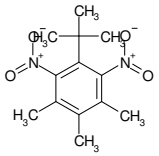
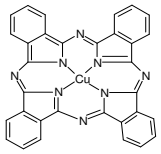
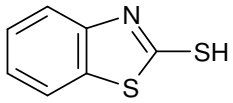
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000123-17-1	5.533843071	-2.404944489	4.48	3.4906571	557.7	2.746
000123-48-8	1.439205604	2.049179787	5.85	0.406532825	6416	3.807
000131-49-7	7.12	-15.94	1.37	17.31	3	0.500
000139-60-6	0.924960236	-5.155574666	7.29	9.051287277	26280	4.420

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000123-17-1	Highly branched P?	neutral	N	Y	
000123-48-8	Highly branched - P but double bond might be reactive	neutral	N	Y	
000131-49-7	Meglumine Diatrizoate. See also 11796May be analysable by GC-MS after derivatization	acid	N	N	Y
000139-60-6	Might be P - highly branched. High predicted B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000123-17-1				N		1	10	10	
000123-48-8				N	0.5	0.5	0.5	0.5	0.5
000131-49-7				N					
000139-60-6				N	0.5	0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000123-17-1		Y	0.162	Mysid Shrimp 96-hour LC50 (mg/L)	
000123-48-8		Y	0.003	Mysid Shrimp 96-hour LC50 (mg/L)	
000131-49-7		N	2510.365	Fish 96-hour LC_{50} (mg/L)	Low
000139-60-6		Y	0.000132	Mysid Shrimp 96-hour LC50 (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000123-17-1	123171	airbreather	Neutral Organics
000123-48-8	123488	MPV	Phenols
000131-49-7	131497		amine
000139-60-6	139606	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000140-66-9	140669	
	000145-39-1	145391	
	000147-14-8	147148	
	000149-30-4	149304	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000140-66-9	Oc(ccc(c1)C(CC(C)(C)C)(C)C)c1	Non-halo	5.18E-04	6.91E-02
000145-39-1	N(=O)(=O)c(c(c(N(=O)(=O))c(c1C)C)C(C)(C)C)c1C	Non-halo	4.36E-06	5.81E-04
000147-14-8	[Cu]6N2C3=Nc8nc(c0c8cccc0)=Nc9c5ccccc5c(n69)N=c7nc(c4c7cccc4)N=C2c1c3cccc1	Non-halo	4.55E-21	6.07E-19
000149-30-4	N(c(c(S1)ccc2)c2)=C1S	Non-halo	4.21E-05	5.61E-03

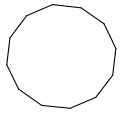
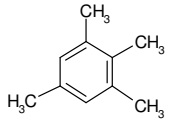
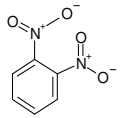
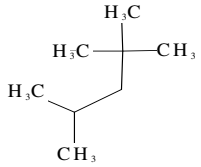
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000140-66-9	0.25	-3.74	5.28	9.02	2303	3.362
000145-39-1	7.27	-4.92	5.18	10.10	1943	3.288
000147-14-8	0.05	-15.86	4.95	20.81	1290	3.111
000149-30-4	0.26	-5.83	2.86	8.69	15	1.163

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000140-66-9	Highly branced octylphenol - similar to nonylphenol??	phenol	N	N	Y
000145-39-1	Not HPV but it looks P - two nitro groups and 1 t-butyl, and 3 methyl - search for nitro musks.	neutral	N	Y	
000147-14-8	Copper phthalocyanine. Pigment. copper ligand - 10-50M every years. May be occupational measurements	neutral	N	N	
000149-30-4	Na salt is in antifreeze - direct release. P but not B. Some used to synthesize vulcanizing agents for rubber - degrades back to mercaptobenzothiazole.	phenol	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000140-66-9	Y			N	50	50	100	50	50
000145-39-1				N	0.5	0.5	0.5		
000147-14-8	?			N	50	50	50	50	50
000149-30-4				N	50	50	50	50	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000140-66-9		Y	2.89E-01	Fish 96-hour LC_{50} (mg/L)	Low
000145-39-1		Y	0.07	Fish 96-hour LC_{50} (mg/L)	Low-moderate
000147-14-8		N	2.50E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000149-30-4		Y	5.834	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000140-66-9	140669		Dinitrobenzenes
000145-39-1	145391		Neutral Organics + Ureas(substituted)
000147-14-8	147148		Triazines
000149-30-4	149304		Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000294-62-2	294622	
	000527-53-7	527537	
	000528-29-0	528290	
	000540-84-1	540841	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000294-62-2	C(CCCCCCCCCC1)C1	Non-halo	2.34E-02	3.12E+00
000527-53-7	c(cc(c(c1C)C)C)(c1)C	Non-halo	3.99E-01	5.32E+01
000528-29-0	O=N(=O)c1ccccc1N(=O)=O	Non-halo	8.85E-05	1.18E-02
000540-84-1	C(CC(C)C)(C)(C)C	Non-halo	4.46E+01	5.95E+03

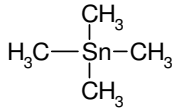
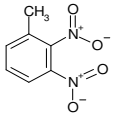
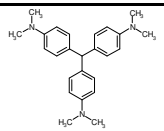
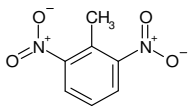
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000294-62-2	0.63	1.76	6.12	4.36	10330	4.014
000527-53-7	0.25	-0.49	4.18	4.67	286	2.457
000528-29-0	502.39	-5.46	1.63	7.09	4	0.601
000540-84-1	2.31	2.09	4.09	2.00	279	2.446

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000294-62-2	Cyclododecane. Widely used solvent. P?? Analysable with other hydrocarbons.	neutral	N	Y	
000527-53-7	tetramethylbenzene; use as solvent, P? Analysable with other hydrocarbons.	neutral	N	Y	
000528-29-0	Dinitrobenzene	neutral	N	Y	
000540-84-1	Trimethylpentane - widely used solvent. Analysable with other hydrocarbons.	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000294-62-2				N	50	50	50	100	100
000527-53-7				N			10		10
000528-29-0				N					
000540-84-1				N	0.5	10	10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000294-62-2		Y	2.55E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000527-53-7		Y	6.80E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000528-29-0		Y	1.43E+00	Fish 96-hour LC_{50} (mg/L)	High-moderate
000540-84-1		Y	6.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000294-62-2	294622		Neutral Organics
000527-53-7	527537		Aliphatic amine + Vinyl/Allyl Halides
000528-29-0	528290		Esters + Vinyl/Allyl Halides
000540-84-1	540841		Benzyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000594-27-4	594274	
	000602-01-7	602017	
	000603-48-5	603485	
	000606-20-2	606202	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000594-27-4	C[Sn](C)(C)C	Non-halo	1.04E+02	1.39E+04
000602-01-7	O=N(=O)c(c(N(=O)=O)c(cc1)C)c1	non-halo	0.00215	0.286643092
000603-48-5	N(c(ccc(c1)C(c(ccc(N(C)C)c2)c2)c(ccc(N(C)C)c3)c3)c1)(C)C	non-halo	5.05E-09	6.73278E-07
000606-20-2	N(=O)(=O)c(c(c(N(=O)(=O))cc1)C)c1	non-halo	0.000806	0.107457829

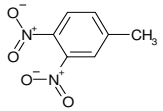
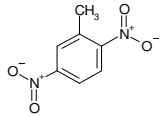
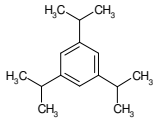
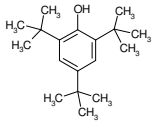
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000594-27-4	1.97	-0.08	3.48	3.56	2397	3.380
000602-01-7	669.975411	-5.421959789	2.18	4.207672401	9.447	0.975
000603-48-5	0.612615522	-8.195446178	5.9	10.70115879	6959	3.843
000606-20-2	595.6131455	-5.421959789	2.18	4.207672401	8.26	0.917

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000594-27-4	Tetramethyltin	neutral	N	Y	
000602-01-7	P? 2 nitro	neutral	N	Y	
000603-48-5	Tert amine P, Kow - B	neutral	N	Y	
000606-20-2	P? 2 nitro	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000594-27-4				N			0.5		
000602-01-7				N	10	10	10		
000603-48-5				N	0.5	0.5	0.5	0.5	0.5
000606-20-2				N	100	500	500		

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000594-27-4		Y	5.40E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000602-01-7		Y	4.138	Fish 96-hour LC_{50} (mg/L)	High-moderate
000603-48-5		Y	0.007	Mysid Shrimp 96-hour LC_{50} (mg/L)	High-moderate
000606-20-2		Y	4.138	Fish 96-hour LC_{50} (mg/L)	moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000594-27-4	594274		Esters + Esters (phosphate)
000602-01-7	602017	airbreather	Esters + Esters (phosphate)
000603-48-5	603485	MPV	Imides
000606-20-2	606202	airbreather	Halopyridine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000610-39-9	610399	
	000619-15-8	619158	
	000717-74-8	717748	
Top 10 non-halogenated	000732-26-3	732263	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000610-39-9	O=N(=O)c(c(N(=O)=O)ccc1C)c1	non-halo	0.00223	0.297308882
000619-15-8	O=N(=O)c(ccc(N(=O)=O)c1C)c1	non-halo	0.00254	0.338638816
000717-74-8	CC(C)c1cc(C(C)C)cc(C(C)C)c1	Non-halo	5.14E-02	6.85E+00
000732-26-3	Oc(c(cc(c1)C(C)(C)C)C(C)(C)C)c1C(C)(C)C	Non-halo	2.00E-04	2.67E-02

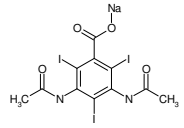
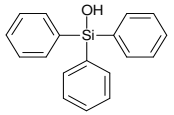
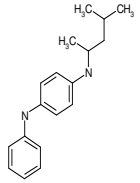
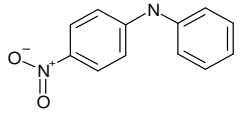
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000610-39-9	669.975411	-5.421959789	2.18	4.207672401	7.973	0.902
000619-15-8	669.975411	-5.421959789	2.18	4.207672401	9.447	0.975
000717-74-8	0.33	0.21	6.36	6.15	15780	4.198
000732-26-3	0.67	-3.40	6.39	9.79	3282	3.516

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000610-39-9	P? dinitrotoluenes? should be some data	neutral	N	Y	
000619-15-8	P? dinitrotoluene	neutral	N	Y	
000717-74-8	1,3,5-Triisopropylbenzene. Use - chemical intermediate and solvent? Analysable with other hydrocarbons/substituted benzenes by GC-MS	neutral	N	Y	
000732-26-3	2,4,6-Tri-tert-butylphenol ; experimental P, like BHT oxidize to quinone?	phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000610-39-9				N	50	50	50		
000619-15-8				N	10	10	10		
000717-74-8				N		0.5	0.5	10	1
000732-26-3				N	10	10	10	10	50

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000610-39-9		Y	4.138	Fish 96-hour LC_{50} (mg/L)	High-moderate
000619-15-8		Y	4.138	Fish 96-hour LC_{50} (mg/L)	moderate
000717-74-8		Y	1.55E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000732-26-3		Y	0.024	Fish 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000610-39-9	610399	airbreather	Neutral Organics
000619-15-8	619158	airbreather	Imides
000717-74-8	717748		Vinyl/Allyl Halides
000732-26-3	732263		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000737-31-5	737315	
	000791-31-1	791311	
	000793-24-8	793248	
	000836-30-6	836306	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000737-31-5	CC(=O)Nc1c(I)c(C(=O)O[Na])c(I)c(NC(=O)C)c1I	Non-halo	3.47E-20	4.63E-18
000791-31-1	O[Si](c1ccccc1)(c2ccccc2)c3ccccc3	non-halo	5.62E-09	7.49272E-07
000793-24-8	N(c(ccc(Nc(cccc1)c1)c2)c2)C(CC(C)C)C	Non-halo	4.93E-06	6.57E-04
000836-30-6	N(=O)(=O)c(ccc(Nc(cccc1)c1)c2)c2	non-halo	0.0000114	0.001519875

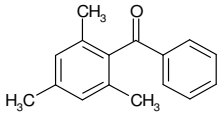
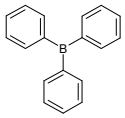
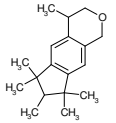
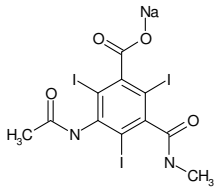
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000737-31-5	7.61	-15.94	-1.28	14.66	3	0.500
000791-31-1	13.80291144	-6.316688769	4.79	7.71240138	977.6	2.990
000793-24-8	0.05	-6.86	4.68	11.54	801	2.904
000836-30-6	0.778550847	-6.771570435	3.69	7.067283046	151.3	2.180

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000737-31-5	see 117964	acid	N	N	Y
000791-31-1	P? Check stability of siloxanes. Check accuracy of Kow estimate	neutral	N	N	Y
000793-24-8	some branching, phenylene diamine - LOGKOW 4.68 Prod last four years 50-100M. There are quite a few like this (e.g., 003081-01-4, 003081-14-9)	neutral	N	Y	
000836-30-6	P? one nitro, check persistence of diphenylamine	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000737-31-5				N					
000791-31-1				N	0.5	0.5	0.5	0.5	0.5
000793-24-8				N	50	100	100	100	100
000836-30-6				N	50	50	50	50	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000737-31-5		N	32320.383	Fish 96-hour LC_{50} (mg/L)	Low
000791-31-1		Y	0.101	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000793-24-8		N	2.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
000836-30-6		Y	1.621	Mysid Shrimp 96-hour LC_{50} (mg/L)	moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000737-31-5	737315		Neutral Organics
000791-31-1	791311	airbreather	Benzyl Halides
000793-24-8	793248		Benzyl Halides
000836-30-6	836306	airbreather	Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000954-16-5	954165	
Top 10 non-halogenated	000960-71-4	960714	
Top 10 non-halogenated	001222-05-5	1222055	
	001225-20-3	1225203	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000954-16-5	O=C(c1c(cc(cc1C)C)C)c2ccccc2	non-halo	0.0000412	0.005492882
000960-71-4	c1ccc(cc1)B(c2ccccc2)c3ccccc3	Non-halo	2.47E-05	3.29E-03
001222-05-5	O(CC(c(c1cc(c2C(C3C)(C)C)C3(C)C)c2)C)C1	Non-halo	8.81E-05	1.17E-02
001225-20-3	CC(=O)Nc1c(I)c(C(=O)O[Na])c(I)c(C(=O)NC)c1I	Non-halo	2.58E-21	3.44E-19

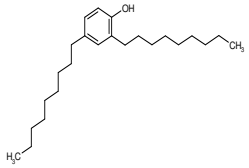
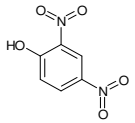
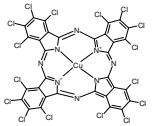
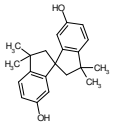
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000954-16-5	3.796561016	-3.971930269	4.79	5.36764288	140.5	2.148
000960-71-4	1.83	-3.00	5.52	8.52	3558	3.551
001222-05-5	0.28	-2.27	6.26	8.53	13200	4.121
001225-20-3	1.67	-16.04	-1.18	14.86	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000954-16-5	P? trimethyl would be stable but maybe not the benzene ring. Photolysis?	neutral	N	Y	
000960-71-4	Check stability of boranes	neutral	N	Y	
001222-05-5	Galoxolide. Highly branched cyclopentyl ring fused on benzene - musk? Use? LOGKOW 6.26 - could be P	neutral	N	Y	
001225-20-3	Iothalamate sodium. Radio contrast agent . See also 117964 and 737315	acid	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000954-16-5				N					0.5
000960-71-4				N	10	10	10	50	10
001222-05-5				N	1	10	10	10	10
001225-20-3				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000954-16-5		Y	0.083	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000960-71-4		Y	2.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001222-05-5		Y	7.37E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001225-20-3		N	27333.012	Fish 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000954-16-5	954165	airbreather	Neutral Organics
000960-71-4	960714		Neutral Organics
001222-05-5	1222055		Neutral Organics
001225-20-3	1225203		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001323-65-5	1323655	
	001326-82-5	1326825	
	001328-53-6	1328536	
	001568-80-5	1568805	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001323-65-5	Oc1ccc(cc1CCCCCCCCC)CCCCCCCCC	Non-halo	1.07E-08	1.43E-06
001326-82-5	O=N(=O)c1cc(ccc1O)N(=O)=O	Non-halo	1.29E-05	1.72E-03
001328-53-6	c12c(c(c(c(c1c1nc3c4c(c(c(c(c4c4n3[Cu]35[n+]1c2nc1n3c(nc2[n+]5c(n4)c3c(c(c(c(c32)Cl)Cl)Cl)Cl)c2c(c(c(c(c21)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl	Non-halo	1.92E-29	2.56E-27
001568-80-5	CC1(CC2(c3cc(ccc3C(C2)(C)C)O)c4cc(ccc14)O)C	non-halo	2.08E-09	2.77311E-07

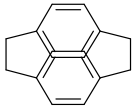
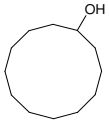
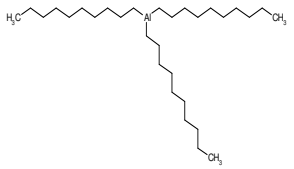
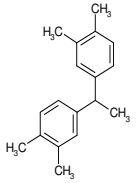
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
001323-65-5	0.15	-2.59	10.47	13.06	3	0.500
001326-82-5	16.19	-5.95	1.73	7.68	4	0.586
001328-53-6	0.51	-12.83	13.60	26.43	3	0.500
001568-80-5	0.717390629	-9.560555712	6.26	12.42626832	13070	4.116

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001323-65-5	Di-Nonylphenol. Highly branched cyclopentyl ring fused on benzene - musk? Use? LOGKOW 6.26 - could be P	phenol	N	N	Y
001326-82-5	Pigment and dye - Sulphur Black 1. May be P but not B. May be amenable to GC after derivatization	phenol	N	N	Y
001328-53-6	Phthalocyanine Green. Pigment/dye. Copper chelate - has four benzene rings with 4 Cl's on each ring - persistent metabolites?	neutral	N	N	
001568-80-5	Maybe P & B	phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001323-65-5				N	10	10	10	0.5	10
001326-82-5				N	10	0.5	10	10	10
001328-53-6	Y?			N	10	10	10	10	10
001568-80-5				N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001323-65-5		N	3.27E-05	Fish 96-hour LC_{50} (mg/L)	Low
001326-82-5		Y	1.03E+01	Fish 96-hour LC_{50} (mg/L)	Moderate
001328-53-6		N	7.65E-13	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001568-80-5		Y	0.094	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
001323-65-5	1323655		Phenols
001326-82-5	1326825		Neutral Organics
001328-53-6	1328536		Neutral Organics
001568-80-5	1568805	MPV	Acid Chloride/Halide

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001633-22-3	1633223	
	001724-39-6	1724396	
	001726-66-5	1726665	
Top 10 non-halogenated	001742-14-9	1742149	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001633-22-3	c(ccc(c1)CCc(ccc(c2)C3)c2)(c1)C3	non-halo	0.000166	0.022131513
001724-39-6	OC(CCCCCCCCCC1)C1	Non-halo	1.25E-04	1.67E-02
001726-66-5	CCCCCCCCCC[Al](CCCCCCCCCC)CCCCCCCCCC	Non-halo	4.47E-10	5.96E-08
001742-14-9	c(ccc(c1C)C)(c1)C(c(ccc(c2C)C)c2)C	Non-halo	7.25E-05	9.67E-03

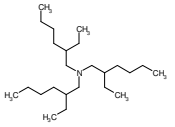
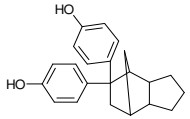
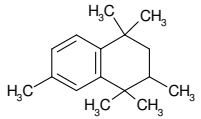
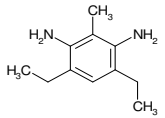
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
001633-22-3	7.826421367	-1.85454467	5.72	4.180257282	5075	3.705
001724-39-6	0.41	-2.96	4.58	7.54	676	2.830
001726-66-5	0.16	1.87	15.23	13.36	3	0.500
001742-14-9	0.33	-1.41	6.34	7.75	15170	4.181

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001633-22-3	May bioaccumulate or not	neutral	N	Y	
001724-39-6	Cyclododecanol . May be relatively persistent?	neutral	N	Y	
001726-66-5	there are a lot of trialkyl aluminums, very high production (10-50M) and LOGKOW values. Stable?? Need to check	neutral	N	N	Y?
001742-14-9	highly substituted, P?	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001633-22-3				N			0.5	0.5	
001724-39-6				N	10	50	50	100	100
001726-66-5	Y?			N	50	50	50	50	50
001742-14-9				N			10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001633-22-3		Y	0.006	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001724-39-6		Y	2.30E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001726-66-5		Y	2.80E-15	Mysid Shrimp 96-hour LC_{50} (mg/L)	
001742-14-9		Y	1.92E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
001633-22-3	1633223	MPV	Neutral Organics
001724-39-6	1724396		Acid Chloride/Halide
001726-66-5	1726665		Neutral Organics
001742-14-9	1742149		Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001860-26-0	1860260	
	001943-97-1	1943971	
	002084-69-7	2084697	
	002095-01-4	2095014	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001860-26-0	CCC(CN(CC(CC)CCCC)CC(CC)CCCC)CCCC	non-halo	0.0000101	0.001346556
001943-97-1	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C(C(C(C34)CC5)C5)C3)C4)c1	non-halo	3.03E-10	4.03967E-08
002084-69-7	c(c(ccc1C)C(CC2C)(C)C)(c1)C2(C)C	non-halo	0.00303	0.403966776
002095-01-4	Nc1c(c(c(cc1CC)CC)N)C	non-halo	0.0000694	0.009252572

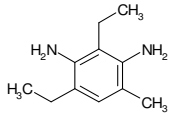
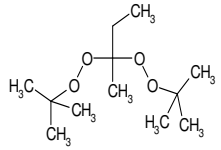
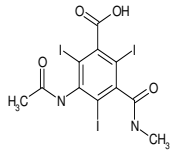
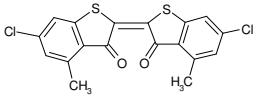
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
001860-26-0	1.024776133	-0.24244274	10.13	6.978155352	3.313	0.520
001943-97-1	1.420639026	-9.63269592	5.42	11.65840853	2991	3.476
002084-69-7	6.837102831	-0.023082791	6.66	3.288795403	27020	4.432
002095-01-4	1.48052761	-7.187173652	2.23	6.022886263	10.46	1.020

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001860-26-0	Branched and tertiary N = P?	neutral	N	Y	
001943-97-1	May be P, related to bis-phenol - A	phenol	N	N	Y
002084-69-7	Polycyclic musk? P & B	neutral	N	Y	
002095-01-4	P?, highly substituted, high previous production	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001860-26-0				N			0.5	0.5	0.5
001943-97-1				N		0.5			
002084-69-7				N		1			
002095-01-4				N			50	10	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001860-26-0		Y	0.000797	Fish 96-hour LC_{50} (mg/L)	
001943-97-1		Y	0.3	Fish 96-hour LC_{50} (mg/L)	
002084-69-7		Y	0.000469	Mysid Shrimp 96-hour LC_{50} (mg/L)	
002095-01-4		Y	29.343	Fish 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
001860-26-0	1860260	MPV	Neutral Organics
001943-97-1	1943971	MPV	Acid Chloride/Halide
002084-69-7	2084697	MPV	Neutral Organics
002095-01-4	2095014	airbreather	Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002095-02-5	2095025	
	002167-23-9	2167239	
	002276-90-6	2276906	
	002379-74-0	2379740	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002095-02-5	Nc1c(c(c(cc1C)CC)N)CC	non-halo	0.0000694	0.009252572
002167-23-9	O(OC(C)(C)C)C(OOC(C)(C)C)(CC)C	Non-halo	1.06E-01	1.41E+01
002276-90-6	CC(=O)Nc1c(I)c(C(=O)O)c(I)c(C(=O)NC)c1I	Non-halo	3.57E-15	4.76E-13
002379-74-0	O=C(c(c(S1)cc(c2)Cl)c2C)C1=C(Sc(c3c(cc4Cl)C)c4)C3=O	non-halo	8.1E-11	1.07991E-08

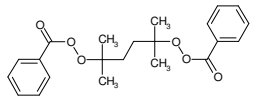
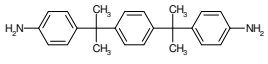
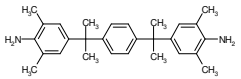
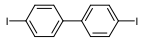
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002095-02-5	1.48052761	-7.187173652	2.23	6.022886263	10.46	1.020
002167-23-9	4.30	-2.47	5.41	7.88	2901	3.463
002276-90-6	1.58	-16.04	1.47	17.51	3	0.500
002379-74-0	2.298880474	-10.90427094	5.92	13.42998355	1035	3.015

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002095-02-5	P?, highly substituted, high previous production	neutral	N	Y	
002167-23-9	Likely amenable to GC analysis	neutral	N	Y	
002276-90-6	Iothalamic Acid. Radiocontrast chemical. See 117964 and 737315	acid	N	N	
002379-74-0	Could be P & B. Use??Rubber chemical?	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002095-02-5				N			50	50	0.5
002167-23-9				N	0.5				
002276-90-6	Y?			N	0.5	0.5	0.5	0.5	0.5
002379-74-0				N	0.5	0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002095-02-5		Y	29.343	Fish 96-hour LC_{50} (mg/L)	Marginal
002167-23-9		Y	0.237	Fish 96-hour LC_{50} (mg/L)	
002276-90-6		N	3756.81	Fish 96-hour LC_{50} (mg/L)	Low
002379-74-0		Y	0.501	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
002095-02-5	2095025	airbreather	neutral Organics
002167-23-9	2167239		Neutral Organics
002276-90-6	2276906		amine + Phenols
002379-74-0	2379740	MPV	Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002618-77-1	2618771	
	002716-10-1	2716101	
	002716-12-3	2716123	
	003001-15-8	3001158	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002618-77-1	O=C(OOC(CCC(OOC(=O)c(cccc1)c1)(C)C)(C)C)c(cccc2)c2	Non-halo	2.14E-07	2.85E-05
002716-10-1	NC3(=CC=C(C(C)(C)C2(=CC=C(C(C)(C)C1(=CC=C(N)C=C1))C=C2))C=C3)	non-halo	7.29E-10	9.7192E-08
002716-12-3	NC3(=C(C)C=C(C(C)(C)C2(C=CC(C(C)(C)C1(=CC(C)=C(N)C(C)=C1))=CC=2))C=C3C)	non-halo	2.67E-11	3.55971E-09
003001-15-8	c(ccc(c(ccc(c1)I)c1)c2)(c2)I	Non-halo	2.06E-06	2.75E-04

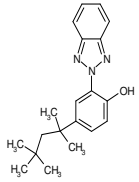
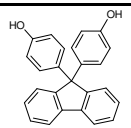
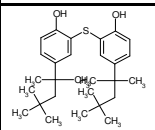
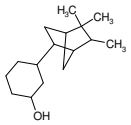
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002618-77-1	1.52	-5.51	5.44	10.95	3078	3.488
002716-10-1	0.639662921	-9.168462688	5.38	11.1541753	2770	3.442
002716-12-3	1.254800563	-8.997635669	7.57	13.17334828	10730	4.031
003001-15-8	6.49	-4.04	6.09	10.13	40770	4.610

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002618-77-1	Chemical intermediate - rubber production? May be amenable to GC analysis although peroxide will degrade	neutral	N	Y?	
002716-10-1	P & B	neutral	N	Y?	
002716-12-3	P & B	neutral	N	Y?	
003001-15-8	Dibenziodolium iodide. Chemical intermediate. May be amenable to GC analysis as with bromobiphenyls	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002618-77-1				N	0.5	0.5	0.5	0.5	
002716-10-1				N		0.5	0.5	0.5	0.5
002716-12-3				N		0.5			
003001-15-8				N	0.5	0.5	0.5		0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002618-77-1		Y	0.207	Fish 96-hour LC_{50} (mg/L)	
002716-10-1		Y	0.867	Fish 96-hour LC_{50} (mg/L)	Low
002716-12-3		Y	0.073	Fish 96-hour LC_{50} (mg/L)	Low
003001-15-8		N	6.70E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
002618-77-1	2618771		Esters
002716-10-1	2716101	MPV	Neutral Organics
002716-12-3	2716123	MPV	Neutral Organics
003001-15-8	3001158		Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	003147-75-9	3147759	
	003236-71-3	3236713	
	003294-03-9	3294039	
	003407-42-9	3407429	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
003147-75-9	Oc(c(n(nc(c1ccc2)c2)n1)cc(c3)C(CC(C)(C)C)(C)C)c3	Non-halo	1.10E-09	1.47E-07
003236-71-3	OC5(=CC=C(C3(C1(=CC=C(O)C=C1))(C2(=C(C=CC=C2)C4(=C3C=CC=C4)))C=C5)	non-halo	6.11E-13	8.146E-11
003294-03-9	Oc(c(Sc(c(O)ccc1C(CC(C)(C)C)(C)C)c1)cc(c2)C(CC(C)(C)C)(C)C)c2	non-halo	2.09E-12	2.78644E-10
003407-42-9	OC(CCCC1C(C(CC2C3(C)C)C3C)C2)C1	non-halo	0.0000122	0.001626533

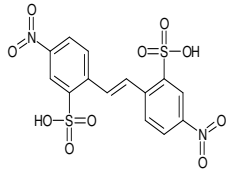
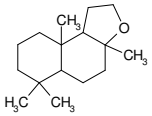
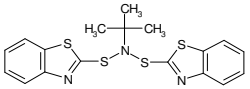
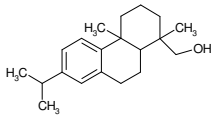
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
003147-75-9	0.33	-10.74	6.21	16.95	12140	4.084
003236-71-3	1.452526928	-12.31668877	6.08	15.00240138	9524	3.979
003294-03-9	2.381948583	-9.048126661	10.86	16.51383927	3.162	0.500
003407-42-9	4.456022632	-3.179055761	5.5	5.284768373	3445	3.537

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
003147-75-9	Branched nonylphenol attached to benzotriazole - looks persistent, LOGKOW 6.21	neutral	N	N	Y
003236-71-3	Maybe P - phenols may biodeg. Potential B	phenol	N	N	Y
003294-03-9	Nonylphenol analog. May not be P	phenol	N	N	Y
003407-42-9	Natural product. May not be P. Kow suggests B	neutral	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
003147-75-9				N	1	10	0.5	10	10
003236-71-3				N		0.5	0.5		
003294-03-9				N	1	0.5	0.5	0.5	
003407-42-9				N		0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
003147-75-9		Y	4.30E-02	Fish 96-hour LC_{50} (mg/L)	
003236-71-3		Y	0.136	Fish 96-hour LC_{50} (mg/L)	
003294-03-9		N	0.000275	Fish 96-hour LC_{50} (mg/L)	
003407-42-9		Y	0.012	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
003147-75-9	3147759		Neutral Organics
003236-71-3	3236713	MPV	Neutral Organics
003294-03-9	3294039	MPV	Neutral Organics
003407-42-9	3407429	MPV	Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	003709-43-1	3709431	
	003738-00-9	3738009	
	003741-80-8	3741808	
	003772-55-2	3772552	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
003709-43-1	S(=O)(=O)(O[Na])c2cc(N(=O)=O)ccc2C=Cc1c(S(=O)(=O)O[Na])cc(N(=O)=O)cc1	Non-halo	5.41E-21	7.21E-19
003738-00-9	O(C(C(C(C(C(CC1)(C)C)C2)(C1)C)C3)(C2)C)C3	non-halo	0.00393	0.523956908
003741-80-8	CC(N(Sc1nc2c(s1)cccc2)Sc3nc4c(s3)cccc4)(C)C	Non-halo	9.34E-12	1.25E-09
003772-55-2	OCC(C(C(c(c(cc(c1)C(C)C)C2)c1)(CC3)C)C2)(C3)C	non-halo	7.87E-08	1.04925E-05

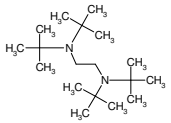
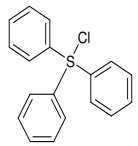
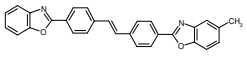
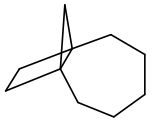
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
003709-43-1	0.06	-19.76	-2.52	17.24	3	0.500
003738-00-9	4.60176057	-1.697489284	4.76	3.063201895	917.3	2.963
003741-80-8	0.12	-12.78	4.15	16.93	311	2.493
003772-55-2	4.144548004	-4.324112787	6.29	7.219825398	3136	3.496

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
003709-43-1	Disodium 4,4'-dinitro-2,2'-stilbenedisulfonate, flourescent brightener. Looks very P but definitely not B. Production 10-50M. May be amenable to LC-MS analysis	acid	N	N	
003738-00-9	P & B - natural product? - may biodeg	neutral	N	Y	
003741-80-8	Benzothiazolesulfenamides are used as rubber vulcanizing agents - 1-10M in 2002. May be amenable to GC anlaysis. Could degrade to loss the amide.	neutral	N	Y?	
003772-55-2	P & B - steroid? May biodeg	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
003709-43-1	Y			N	10	10	10	50	50
003738-00-9				N				0.5	0.5
003741-80-8		Benzothiazolesulfenamide	?	N			1		10
003772-55-2				N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
003709-43-1		Y	3.50E+06	Fish 96-hour LC_{50} (mg/L)	
003738-00-9		Y	0.095	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003741-80-8		N	1.77E-01	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003772-55-2		Y	0.00171	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
003709-43-1	3709431		Acid Chloride/Halide + Vinyl/Allyl Ethers
003738-00-9	3738009	MPV	Acrylates
003741-80-8	3741808		Neutral Organics
003772-55-2	3772552	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	004062-60-6	4062606	
	004270-70-6	4270706	
	005242-49-9	5242499	
	6004-38-2	6004382	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
004062-60-6	N(C(C)(C)C)CCNC(C)(C)C	non-halo	0.35	46.66282895
004270-70-6	c(ccc1)c(c1)S(Cl)(c(ccc2)cc2)c(ccc3)cc3	Non-halo	6.78E-07	9.04E-05
005242-49-9	n1c2ccccc2oc1c3ccc(C=Cc4ccc(c5oc6ccc(C)cc6n5)cc4)cc3	non-halo	5.45E-14	7.26607E-12
6004-38-2	C2CCC13CCC1(CC2)C3	Non-halo		

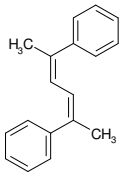
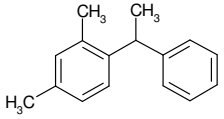
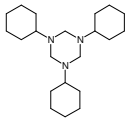
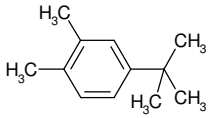
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
004062-60-6	0.865128343	-5.952408129	2.04	4.598120741	7.398	0.869
004270-70-6	8.55	-4.24	7.26	11.50	28320	4.452
005242-49-9	1.330482376	-12.27129948	8.05	16.92701209	2349	3.371
6004-38-2	1.36	6.303370787	4.01		243.7	2.390

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
004062-60-6	This might be quite P	amine	N	Y	
004270-70-6	Triphenyl sulfonium chloride. May be amenable to GC analysis	neutral	N	Y	
005242-49-9	Double bond may be reactive. Use?	neutral	N	Y	
6004-38-2		neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
004062-60-6				N	0.5	0.5		1	1
004270-70-6				N					
005242-49-9				N		0.5	0.5	0.5	0.5
6004-38-2				N					No Reports

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
004062-60-6		Y	28.727	Fish 96-hour LC_{50} (mg/L)	
004270-70-6		N	1.70E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
005242-49-9		N	2.50E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
6004-38-2	>500K - 1M		8.90E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
004062-60-6	4062606	MPV	Dinitrobenzenes
004270-70-6	4270706		Acrylates
005242-49-9	5242499	MPV	Neutral Organics
6004-38-2			Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	006144-04-3	6144043	
	006165-52-2	6165522	
	006281-14-7	6281147	
	007397-06-0	7397060	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
006144-04-3	CC(C=CC(c1ccccc1)C)c2ccccc2	Non-halo	2.56E-04	3.41E-02
006165-52-2	c(cccc1)(c1)C(c(c(cc(c2)C)C)c2)C	non-halo	0.000638	0.085059671
006281-14-7	N4(C1(CCCCC1))(CN(C2(CCCCC2))CN(C3(CCCCC3))C4)	non-halo	0.00000018	2.3998E-05
007397-06-0	c(ccc(c1C)C)(c1)C(C)(C)C	non-halo	0.211	28.13101974

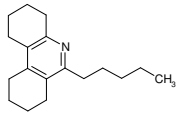
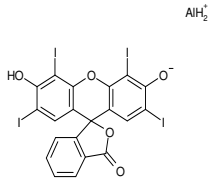
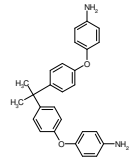
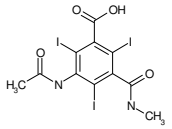
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
006144-04-3	0.06	-1.15	6.34	7.49	15240	4.183
006165-52-2	5.581773696	-1.498709055	5.24	3.344421666	2179	3.338
006281-14-7	0.236205337	-1.634987717	4.66	2.900700329	767.7	2.885
007397-06-0	8.839518236	-0.160684071	5	1.766396683	1405	3.148

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
006144-04-3	a-Methylstyrene Dimer; extended conjugated system - photolysis?, used in order to control the molecular weight in solution polymerizations. May be amenable to GC analysis	neutral	N	Y?	
006165-52-2	Branced/substituted = P. Could be B	neutral	N	Y	
006281-14-7	Tertiary N, acyclic rings = P?	neutral	N	Y	
007397-06-0	Highly substituted & t-butyl group, B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
006144-04-3				N	0.5		1	10	10
006165-52-2				N		0.5			
006281-14-7				N		0.5	0.5		
007397-06-0				N				0.5	1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
006144-04-3		Y	1.90E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
006165-52-2		Y	0.004	Mysid Shrimp 96-hour LC_{50} (mg/L)	
006281-14-7		Y	1.823	Fish 96-hour LC_{50} (mg/L)	
007397-06-0		Y	0.006	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
006144-04-3	6144043		Esters
006165-52-2	6165522	MPV	Aliphatic amine
006281-14-7	6281147	MPV	Neutral Organics
007397-06-0	7397060	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	010594-03-3	10594033	
	012227-78-0	12227780	
	013080-86-9	13080869	
	013087-53-1	13087531	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
010594-03-3	n(c(c(c(c1CCC2)C2)CCC3)C3)c1CCCCC	non-halo	0.0000107	0.001426549
012227-78-0	c42Oc5c(I)c(O)c(I)cc5C3(c4cc(I)c(O)c2I)OC(=O)c1ccccc31	Non-halo	3.93E-20	5.24E-18
013080-86-9	O(c(ccc(c1)C(c(ccc(Oc(ccc(N)c2)c2)c3)c3)(C)C)c1)c(ccc(N)c4)c4	non-halo	1.64E-12	2.18649E-10
013087-53-1	CC(=O)Nc1c(I)c(C(=O)O)c(I)c(C(=O)NC)c1I	Non-halo	3.57E-15	4.76E-13

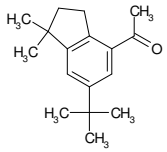
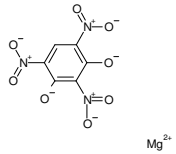
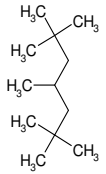
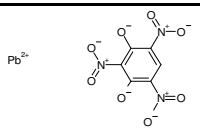
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
010594-03-3	5.356289647	-3.054117025	7.24	6.899829636	29810	4.474
012227-78-0	1.82	-17.98	8.02	26.00	1031	3.013
013080-86-9	0.64073113	-11.6852794	6.88	15.17099201	39730	4.599
013087-53-1	1.58	-16.04	1.47	17.51	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
010594-03-3	Maybe P - straight chain may biodeg. Use?	neutral	N	Y	
012227-78-0	Pigment and dye. May be amenable to LC-MS analysis	phenol	N	N	
013080-86-9	P?? Dye?	neutral	N	Y?	
013087-53-1	Iothalamate sodium. Radio contrast agent . See also 117964 and 737315. May be amenable to LC-MS (ESI) analysis	acid	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
010594-03-3				N	0.5	0.5		1	0.5
012227-78-0	Y?			N	0.5	0.5		0.5	
013080-86-9				N				0.5	0.5
013087-53-1	Y?			N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
010594-03-3			1.55E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
012227-78-0		Y	0.002	Mysid Shrimp 96-hour LC_{50} (mg/L)	
013080-86-9			0.031	Fish 96-hour LC_{50} (mg/L)	
013087-53-1		N	2076.089	Fish 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
010594-03-3	10594033	MPV	Neutral Organics
012227-78-0	12227780		Neutral Organics
013080-86-9	13080869	MPV	Neutral Organics
013087-53-1	13087531		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 non-halogenated	013171-00-1	13171001	
	013255-27-1	13255271	
	013475-82-6	13475826	
	015245-44-0	15245440	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
013171-00-1	O=C(c(c(c(cc1C(C)(C)C)C(C2)(C)C)C2)c1)C	Non-halo	1.44E-04	1.92E-02
013255-27-1	N(=O)(=O)c1c(O[Mg])c(N(=O)=O)c(O)c(N(=O)=O)c1	non-halo	2.32E-09	3.09308E-07
013475-82-6	C(CC(CC(C)(C)C)C)(C)(C)C	Non-halo	1.46E+00	1.95E+02
015245-44-0	N(=O)(=O)c1c(O)c(N(=O)(=O))c(O)c(N(=O)(=O))c1	non-halo	2.65E-09	3.53304E-07

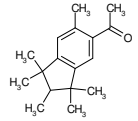
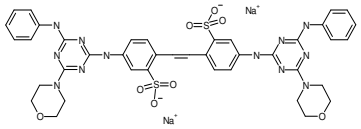
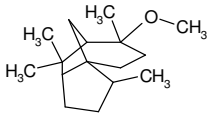
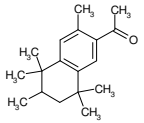
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
013171-00-1	1.44	-2.75	5.93	8.68	1057	3.024
013255-27-1	911.8461959		0.28		3.162	0.500
013475-82-6	1.54	2.58	5.94	3.36	7464	3.873
015245-44-0	457.4178212	-8.834687749	1.06	6.500400361	1.315	0.119

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
013171-00-1	musk dimethyl indane	neutral	Y	Y	
013255-27-1	Several trinitro salts P? Probably not B Use? Explosives?	phenol	N	N	Y
013475-82-6	2,2,4,6,6-pentamethyl-heptane. Solvent. May be persistent in ground water.	neutral	N	Y	
015245-44-0	Tri NO2 - several of these. Use?	Phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
013171-00-1				Y	0.5	0.5	0.5	0.5	0.5
013255-27-1				N	0.5	0.5	0.5	0.5	0.5
013475-82-6				N		0.5	0.5	1	0.5
015245-44-0				N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
013171-00-1		Y	6.39E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
013255-27-1			97.5	Fish 96-hour LC_{50} (mg/L)	
013475-82-6		Y	4.33E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
015245-44-0			32.5	Fish 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
013171-00-1	13171001		Aliphatic amine
013255-27-1	13255271	MPV	Methacrylates
013475-82-6	13475826		Neutral Organics
015245-44-0	15245440	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	015323-35-0	15323350	
	016090-02-1	16090021	
	019870-74-7	19870747	
	021145-77-7	21145777	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
015323-35-0	O=C(c(c(cc(c1C(C2C)(C)C)C2(C)C)C)c1)C	Non-halo	1.47E-04	1.96E-02
016090-02-1	OS(=O)(=O)c2c(ccc(c2)Nc3nc(nc(n3)Nc4ccccc4)N5CCOCC5)C=Cc6ccc(cc6S(=O)(=O)O)Nc7nc(nc(n7)Nc8ccccc8)N1CCOCC1	Non-halo	2.25E-38	3.00E-36
019870-74-7	O(C(C(CC(C1CC2)(C2C)C3)C1(C)C)(C3)C)C	non-halo	0.00915	1.219899671
021145-77-7	O=C(c(c(cc(c1C(CC2C)(C)C)C2(C)C)C)c1)C	Non-halo	5.57E-05	7.43E-03

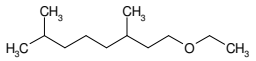
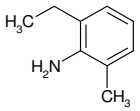
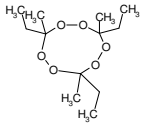
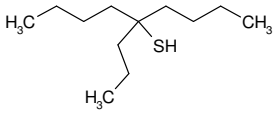
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
015323-35-0	0.70	-2.89	5.85	8.74	928	2.968
016090-02-1	0.02	-41.47	5.95	47.42	6	0.750
019870-74-7	6.454828426	-0.797506169	5.03	2.433218781	1477	3.169
021145-77-7	0.60	-2.76	6.35	9.11	2217	3.346

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
015323-35-0	musk indane. Analysable with other hydrocarbons/substituted benzenes by GC-MS	neutral	Y	Y	
016090-02-1	Fluorescent Whitening Agent (FWA) mainly used (more than 90%) in household detergents in concentrations ranging from 0.05 to 0.15%. Example of many dyes and pigments,produced in high vol, hig Kow but have such high MW (924) unlikely to be B - probably per	acid	N	N	
019870-74-7	P & B - ether stable. Musk	neutral	N	Y	
021145-77-7	Synthetic musk AHTN, 7-acetyl-1,1,3,4,4,-hexamethyl tetrahydronaphthalene. Analysable by GC-MS. Measurements for the Great Lakes	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
015323-35-0				Y					
016090-02-1	Y?			N	10	10	10	50	10
019870-74-7				N		0.5	0.5	0.5	0.5
021145-77-7				Y	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
015323-35-0		Y	8.05E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
016090-02-1		Y	1.27E+00	Fish 96-hour LC_{50} (mg/L)	
019870-74-7			0.008	Mysid Shrimp 96-hour LC_{50} (mg/L)	
021145-77-7		Y	1.31E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
015323-35-0	15323350		Surfactants-cationic
016090-02-1	16090021		Neutral Organics
019870-74-7	19870747	MPV	Neutral Organics
021145-77-7	21145777		Esters

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	022810-10-2	22810102	
	024549-06-2	24549062	
	024748-23-0	24748230	
	025103-58-6	25103586	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
022810-10-2	O(CCC(CCCC(C)C)C)CC	non-halo	0.461	61.46161184
024549-06-2	Nc(c(ccc1)CC)c1C	non-halo	0.0742	9.892519737
024748-23-0	O1OC(OOC(OOC1(C)CC)(C)CC)(C)CC	Non-halo	4.75E-04	6.33E-02
025103-58-6	SC(CCC)(CCCC)CCCC	Non-halo	2.52E-02	3.36E+00

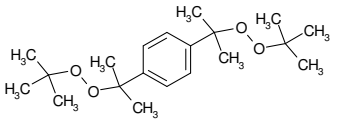
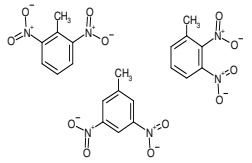
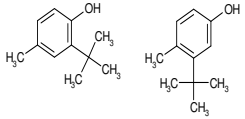
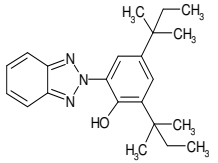
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
022810-10-2	4.708013158	-0.221253441	4.83	1.656966053	1047	3.020
024549-06-2	0.792322953	-3.900020059	2.66	3.165732671	22.36	1.349
024748-23-0	2.40	-4.48	6.10	10.58	9984	3.999
025103-58-6	0.25	0.38	6.07	5.69	296	2.472

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
022810-10-2	P & B - low B	neutral	N	Y	
024549-06-2		neutral	N	Y	
024748-23-0	Used as a plastics modifier, not to exceed 0.15%, of olefin polymers for single and repeat-use food contact applications. Probably analysable by GC-MS	neutral	N	Y	
025103-58-6	tert-dodecanethiol. Modifier of mol weight distribution in synthetic rubber and latex. UK Environ Risk asssessment. Likely can be analysed by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
022810-10-2				N			0.5		
024549-06-2				N	10	10	50	50	50
024748-23-0				N				0.5	
025103-58-6				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
022810-10-2		Y	0.012	Mysid Shrimp 96-hour LC_{50} (mg/L)	
024549-06-2			13.2	Fish 96-hour LC_{50} (mg/L)	High-moderate
024748-23-0		Y	1.35E+00	Fish 96-hour LC_{50} (mg/L)	
025103-58-6		Y	0.015	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
022810-10-2	22810102	MPV	Esters
024549-06-2	24549062	airbreather	Phenols
024748-23-0	24748230		Esters + Acid Chloride/Halide
025103-58-6	25103586		Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	025155-25-3	25155253	
	025321-14-6	25321146	 MIXTURE OF ISOMERS
	025567-40-2	25567402	
Top 10 non-halogenated	025973-55-1	25973551	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
025155-25-3	CC(c1ccc(cc1)C(OOC(C)(C)C)(C)C)(OOC(C)(C)C)C	Non-halo	1.71E-05	2.28E-03
025321-14-6	Cc1cccc(N(=O)(=O))c1N(=O)(=O)	Non-halo	2.15E-03	2.87E-01
025567-40-2	CC(c1ccc(cc1)C)(C)C	Non-halo	5.92E-01	7.89E+01
025973-55-1	Oc(c(cc(c1)C(CC)(C)C)C(CC)(C)C)c1n(nc(c2ccc3)c3)n2	Non-halo	1.93E-10	2.57E-08

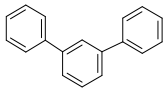
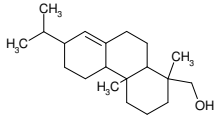
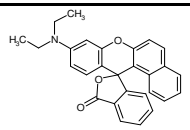
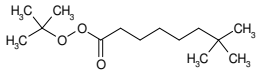
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
025155-25-3	1.57	-2.40	7.34	9.74	22340	4.349
025321-14-6	55.83	-5.42	2.18	7.60	9	0.975
025567-40-2	1.59	-1.20	4.45	5.65	1909	3.281
025973-55-1	0.68	-10.57	7.25	17.82	10350	4.015

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
025155-25-3	Crosslinking agent in polymer production. May be analysable by GC-MS	neutral	N	Y?	
025321-14-6	Di nitro toluene. Not bioaccumulative, but may be persistent - extremely large production. Analysable by GC-MS.	neutral	N	Y	
025567-40-2	1-tert Butyl-4-methyl benzene. Solvent use? Analysable by GC-MS.	neutral	N	N	Y
025973-55-1	UV absorber used in rubber, polymer industry. Likely analysable by GC-MS after derivatization or possibly by LC-MS (ESI)	phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
025155-25-3				N	10	10	10	10	
025321-14-6				N	500	500	500	5000	5000
025567-40-2				N					
025973-55-1				N	10	10	10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
025155-25-3		Y	2.44E+00	Fish 96-hour LC_{50} (mg/L)	
025321-14-6		Y	1.42E+00	Fish 96-hour LC_{50} (mg/L)	High-moderate
025567-40-2		Y	2.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
025973-55-1		Y	0.073	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
025155-25-3	25155253		Neutral Organics
025321-14-6	25321146		Neutral Organics
025567-40-2	25567402		Esters + Silanes (alkoxy)
025973-55-1	25973551		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	026140-60-3	26140603	
	026266-77-3	26266773	
	026628-47-7	26628477	
	026748-41-4	26748414	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
026140-60-3	c1ccc(cc1)c2ccc(cc2)c3ccccc3	Non-halo	3.42E-07	4.56E-05
026266-77-3	OCC(C(C(C(C(=CC(C1)C(C)C)C2)C1)(CC3)C)C2)(C3)C	non-halo	0.000000215	2.86643E-05
026628-47-7	O=C(OC(c(c(Oc1ccc(c2ccc3)c3)cc(N(CC)CC)c4)c4)(c12)c5cccc6)c56	non-halo	4.44E-13	5.91951E-11
026748-41-4	O=C(OOC(C)(C)C)CCCCCC(C)(C)C	Non-halo	8.24E-03	1.10E+00

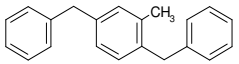
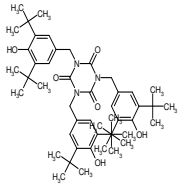
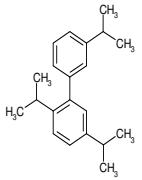
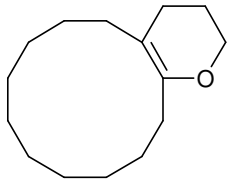
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
026140-60-3	1.16	-2.89	5.52	8.41	8772	3.943
026266-77-3	1.133692814	-2.670900273	6.32	5.596612885	14620	4.165
026628-47-7	0.469342554	-9.036388258	6.65	12.29210087	26190	4.418
026748-41-4	1.53	-0.39	5.25	5.64	2212	3.345

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
026140-60-3	Terphenyl. High boiling hydrocarbon cooling fluid. Analysable with other hydrocarbons.	neutral	Y	Y	
026266-77-3	P & B acyclic, branched = P	neutral	N	Y?	
026628-47-7	Spiro dye intermediate could be P & B	neutral	N	Y?	
026748-41-4	Polymerization Initiator in polymer production. May be analysable by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
026140-60-3				N	10	10	1	50	50
026266-77-3				N				0.5	
026628-47-7				N		0.5	0.5	0.5	
026748-41-4				N	10	10	10	10	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
026140-60-3		Y	1.96E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
026266-77-3		Y	2.47E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
026628-47-7			0.126	Fish 96-hour LC_{50} (mg/L)	
026748-41-4		Y	0.206	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
026140-60-3	26140603		Neutral Organics
026266-77-3	26266773	MPV	Neutral Organics
026628-47-7	26628477	MPV	Neutral Organics
026748-41-4			Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	026898-17-9	26898179	
	027676-62-6	27676626	
	029225-91-0	29225910	
	32539-83-6	32539836	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
026898-17-9	Cc1cc(ccc1Cc2ccccc2)Cc3ccccc3	non-halo	0.00000137	0.000182652
027676-62-6	Oc(c(cc1CN(C(=O)N(C2(=O))Cc(cc(c3O)C(C)(C)C)cc3C(C)(C)C)C(=O)N2Cc(cc(c4O)C(C)(C)C)cc4C(C)(C)C)C(C)(C)C)c(c1)C(C)(C)C	Non-halo	4.68E-28	6.24E-26
029225-91-0	CC(c1ccccc1c2c(cccc2C(C)C)C(C)C)C	Non-halo	9.07E-06	1.21E-03
32539-83-6	C1CCCCCC2=C(CCCC1)CCCO2	Non-halo		

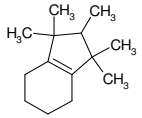
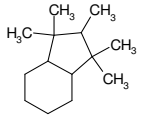
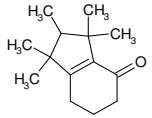
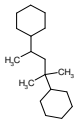
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
026898-17-9	4.735847091	-2.714628777	6.59	5.910341389	23480	4.371
027676-62-6	0.16	-24.18	15.18	39.36	3	0.500
029225-91-0	0.57	-1.91	8.13	10.04	1857	3.269
32539-83-6	0.06	2.247110754	5.78		5649	3.750

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
026898-17-9	P?? B	neutral	N	Y	
027676-62-6	Antioxidant. low discoloration in applications exposed to “gas fade”. environments and/or dark storage. 'Possible degradation product, triazine, might be stable. Hi molecular weight and LOGKOW is 15.18 so parent should not bioaccumulate. Phenol may be ana	phenol	N	N	Y?
029225-91-0	Triisopropylbiphenyl. Three isopropyl groups on a biphenyl may lead to high persistence. Analysable with other hydrocarbons by GC-MS	neutral	N	Y	
32539-83-6		neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
026898-17-9				N	0.5	0.5	0.5	0.5	1
027676-62-6	Y?			N	10	10	10	10	10
029225-91-0				N				0.5	10
32539-83-6				N					No Reports

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
026898-17-9			1.07E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
027676-62-6		N	1.45E-06	Fish 96-hour LC_{50} (mg/L)	
029225-91-0		Y	1.30E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
32539-83-6	>1M - 10M	Y	0.00148	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
026898-17-9	26898179	MPV	Aliphatic amine
027676-62-6			Neutral Organics
029225-91-0			Neutral Organics
32539-83-6			Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	033704-59-5	33704595	
	033704-60-8	33704608	
	033704-61-9	33704619	
	038970-72-8	38970728	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
033704-59-5	C(=C(C(C1C)(C)C)CCC2)(C1(C)C)C2	non-halo	0.0935	12.46564145
033704-60-8	C(C(C(C1C)(C)C)CCC2)(C1(C)C)C2	non-halo	0.207	27.59773026
033704-61-9	O=C(C(=C(C(C1C)(C)C)CC2)C1(C)C)C2	non-halo	0.00403	0.537289145
038970-72-8	C(CCCC1)(C1)C(CC(C(CCCC2)C2)(C)C)C	non-halo	0.00367	0.489293092

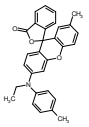
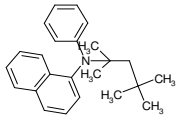
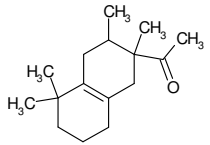
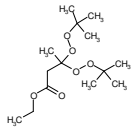
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
033704-59-5	1.089291993	1.205821774	6.25	1.649890837	12990	4.114
033704-60-8	9.883075118	1.648855722	5.87	0.82685689	6548	3.816
033704-61-9	1.186265126	-2.236282432	4.49	3.331995043	572.4	2.758
038970-72-8	4.899154407	2.139059125	8.62	3.086653487	383.7	2.584

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
033704-59-5	P & B. Musk?	neutral	N	Y	
033704-60-8	P & B. Musk?	neutral	N	Y	
033704-61-9	P & B. Musk?	neutral	N	Y	
038970-72-8	Branched and acyclic = P. Could be B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
033704-59-5				N	0.5		0.5	0.5	
033704-60-8				N		0.5		0.5	
033704-61-9				N	0.5	0.5	0.5	0.5	0.5
038970-72-8				N	0.5	0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
033704-59-5		Y	2.00E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
033704-60-8		Y	6.04E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
033704-61-9		Y	0.043	Mysid Shrimp 96-hour LC_{50} (mg/L)	
038970-72-8		N	2.84E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
033704-59-5	33704595	MPV	Triazines + Vinyl/Allyl Ethers
033704-60-8	33704608	MPV	Phenols
033704-61-9	33704619	MPV	Neutral Organics
038970-72-8	38970728	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	042228-32-0	42228320	
	051772-35-1	51772351	
	54464-59-4	54464594	
	055794-20-2	55794202	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
042228-32-0	O=C(OC(c(c(Oc1cc(N(c(ccc(c2)C)c2)CC)cc3)ccc4C)c4)(c13)c5cccc6)c56	non-halo	1.68E-13	2.23982E-11
051772-35-1	CC(CC(C)(C)C)(C)N(c1(ccccc1))c3(c2(c(cccc2)ccc3))	non-halo	0.000000109	1.45321E-05
54464-59-4	CC(=O)C1(C)CC2=C(CC1(C)C)C(C)(C)CCC2	Non-halo		
055794-20-2	O=C(OCC)CC(OOC(C)(C)C)(OOC(C)(C)C)C	Non-halo	6.48E-04	8.64E-02

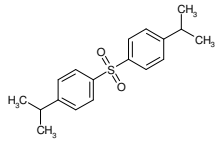
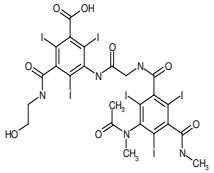
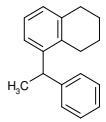
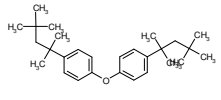
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
042228-32-0	0.613797014	-8.662659144	7.74	13.00837176	6207	3.793
051772-35-1	0.368001813	-3.203879345	8.23	8.039591957	1333	3.125
54464-59-4	0.09	0.0255	5.64		4375	3.640
055794-20-2	3.35	-4.09	4.95	9.04	1285	3.109

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
042228-32-0	Lot of spiro compds. Dye intermediate	neutral	N	Y	
051772-35-1	May be P (tert amine, branching)	neutral	N	Y	
54464-59-4	Fragrances?	neutral	N	Y	
055794-20-2	ethyl 3,3-di(tert-butylperoxy)butyrate. use as hydrolysis stabilizers and vinyl polymerization initiator. May be analysable by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
042228-32-0				N					0.5
051772-35-1				N	0.5		0.5	0.5	
54464-59-4		Y	Y	N					No Reports
055794-20-2				N		0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
042228-32-0			0.002	Mysid Shrimp 96-hour LC_{50} (mg/L)	
051772-35-1			1.16E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
54464-59-4	>500K - 1M		1.50E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
055794-20-2		Y	0.251	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
042228-32-0	42228320	MPV	Halo Benzamides
051772-35-1	51772351	MPV	Neutral Organics
54464-59-4			Neutral Organics
055794-20-2	55794202		Aliphatic amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	057913-35-6	57913356	
	059017-64-0	59017640	
	060466-61-7	60466617	
	061702-88-3	61702883	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
057913-35-6	O=S(=O)(c(ccc(c1)C(C)C)c1)c(ccc(c2)C(C)C)c2	Non-halo	2.91E-07	3.88E-05
059017-64-0	OCCNC(=O)c1c(I)c(C(=O)O)c(I)c(NC(=O)CNC(=O)c2c(I)c(C(=O)NC)c(I)c(N(C)C(=O)C)c2I)c1I	Non-halo	1.83E-39	2.44E-37
060466-61-7	CC(c1cccc2c1CCCC2)c3ccccc3	Non-halo	5.17E-05	6.89E-03
061702-88-3	CC(c1ccc(cc1)Oc2ccc(cc2)C(CC(C)(C)C)(C)C)(CC(C)(C)C)C	non-halo	9.96E-08	1.32789E-05

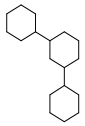
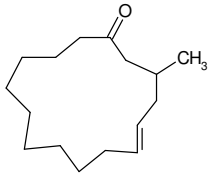
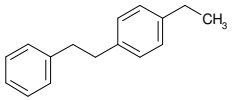
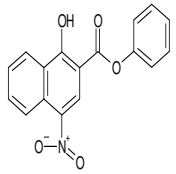
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
057913-35-6	1.64	-4.41	5.52	9.93	3545	3.550
059017-64-0	0.35	-38.82	2.51	41.33	3	0.500
060466-61-7	0.41	-2.61	6.11	8.72	10190	4.008
061702-88-3	7.87268517	-0.50890157	11.57	8.684614182	3.162	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
057913-35-6	bis(p-isopropylphenyl)sulfone. May be analysable by GC-MS similar to other sulfones	neutral	N	Y	
059017-64-0	iopamidol. Radio contrast agent. See also 117964 and 737315. May be amenable to LC-MS (ESI)	neutral	N	N	
060466-61-7	Substituted napthalene. May be persistent. Analysable with other hydrocarbons	neutral	N	Y	
061702-88-3	P (branched although diphenyl oxide biodeg). Maybe B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
057913-35-6				N					
059017-64-0	Y?			N					
060466-61-7				N				0.5	10
061702-88-3				N	0.5				

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
057913-35-6		N	3.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
059017-64-0		Y	6.25E+02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
060466-61-7		Y	3.68E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
061702-88-3			9.20E-11	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
057913-35-6	57913356		Neutral Organics
059017-64-0	59017640		Halo Benzamides
060466-61-7	60466617		Neutral Organics
061702-88-3	61702883	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	061788-32-7	61788327	
	63314-79-4	63314794	
	064800-83-5	64800835	
	065208-34-6	65208346	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
061788-32-7	C1(C2CCCCC2)CCCC(C3CCCCC3)C1	Non-halo	7.53E-04	1.00E-01
63314-79-4	CC1CC=CCCCCCCCCC(=O)C1	Non-halo		
064800-83-5	CCc1ccc(cc1)CCc2ccccc2	non-halo	0.000373	0.049729243
065208-34-6	O=C(Oc(cccc1)c1)c(c(O)c(c(c2N(=O)=O)ccc3)c3)c2	Non-halo	3.52E-10	4.69E-08

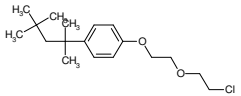
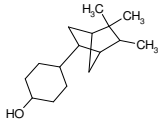
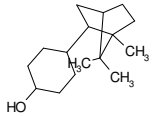
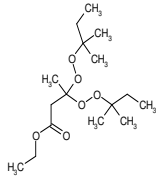
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
061788-32-7	0.31	1.78	8.55	6.77	486	2.686
63314-79-4	0.06	0.0235	5.26		2229	3.350
064800-83-5	9.07345884	-1.4182239	5.78	3.803936511	5607	3.749
065208-34-6	1.54	-8.58	5.39	13.97	2829	3.452

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
061788-32-7	Referred to as Hydrogenated terphenyls. Look very persistent. Should be analysable with hydrocarbons	neutral	N	Y	
63314-79-4	New fragrance Muscenones 3-methylcyclopentadec-5-en-1-ones	neutral	N	Y	
064800-83-5	P? may biodeg. B	neutral	N	Y	
065208-34-6	Use? May be analysable by LC-MS.	phenol	N	N	Y

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
061788-32-7				N	10	10	10	10	50
63314-79-4				N					No Reports
064800-83-5				N	0.5	0.5	1	1	1
065208-34-6	Y?			N	0.5	0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
061788-32-7		Y	3.45E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	
63314-79-4	10K - 500K	Y	4.00E-03	Mysid Shrimp 96-hour LC50 (mg/L)	
064800-83-5		Y	8.47E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
065208-34-6		Y	0.117	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
061788-32-7	61788327		Neutral Organics
63314-79-4			Aliphatic amine
064800-83-5	64800835	MPV	Neutral Organics
065208-34-6	65208346		Esters + Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	065925-28-2	65925282	
	066068-84-6	66068846	
	066072-32-0	66072320	
	067567-23-1	67567231	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
065925-28-2	O(CCOc(ccc(c1)C(CC(C)(C)C)(C)C)c1)CCCl	non-halo	0.0000128	0.001706526
066068-84-6	OC(CCC(C(C(CC1C2(C)C)C2C)C1)C3)C3	non-halo	0.0000122	0.001626533
066072-32-0	OC(CCC(C(C(C(C1C2)(C)C)(C2)C)C1)C3)C3	non-halo	0.0000142	0.001893178
067567-23-1	O=C(OCC)CC(OOC(CC)(C)C)(OOC(CC)(C)C)C	Non-halo	9.55E-05	1.27E-02

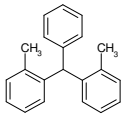
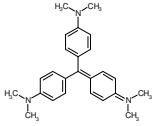
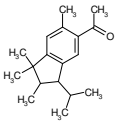
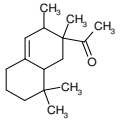
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
065925-28-2	3.249881991	-3.119057832	6.31	6.034770443	14340	4.157
066068-84-6	4.456022632	-3.179055761	5.5	5.284768373	3445	3.537
066072-32-0	4.811314897	-3.179055761	5.54	5.324768373	3671	3.565
067567-23-1	1.95	-3.85	5.93	9.78	7331	3.865

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
065925-28-2	May be P - branching, ethers (maybe not - ethoxylate). B	neutral	N	Y	
066068-84-6	Maybe P (bicyclic and acyclic). B	neutral	N	N	Y
066072-32-0	Maybe P (bicyclic and acyclic), B	neutral	N	N	Y
067567-23-1	Peroxides used as hydrolysis stabilizers and vinyl polymerization initiators. See also 55794-20-2	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
065925-28-2				N	0.5				
066068-84-6				N	0.5	0.5	0.5	0.5	
066072-32-0				N			0.5	0.5	0.5
067567-23-1				N		0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
065925-28-2		Y	0.055	Fish 96-hour LC_{50} (mg/L)	
066068-84-6		Y	0.002	Mysid Shrimp 96-hour LC_{50} (mg/L)	
066072-32-0			0.0019	Mysid Shrimp 96-hour LC_{50} (mg/L)	
067567-23-1		Y	0.045	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
065925-28-2	65925282	MPV	Triazines
066068-84-6	66068846	MPV	Neutral Organics
066072-32-0	66072320	MPV	Peroxy Acids
067567-23-1	67567231		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	067881-18-9	67881189	
	067939-65-5	67939655	
Top 10 non-halogenated	068140-48-7	68140487	
	068155-66-8	68155668	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
067881-18-9	Cc2ccccc2C(c3ccccc3)c1c(cccc1)C	non-halo	0.00000215	0.000286643
067939-65-5	C1(=C(c3ccc(N(C)C)cc3)c2ccc(N(C)C)cc2)C=CC(=N(OC(=O)C)(C)(C))C=C1	non-halo	1.79E-15	2.38647E-13
068140-48-7	O=C(c(c(cc(c1C(C2C)C(C)C)C2(C)C)C)c1)C	Non-halo	6.83E-05	9.11E-03
068155-66-8	O=C(C(C(C=C(C1C(CC2)(C)C)C2)C)(C1)C)C	non-halo	0.00151	0.201316776

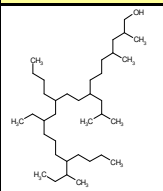
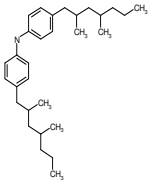
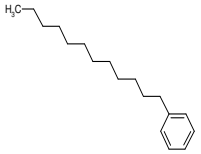
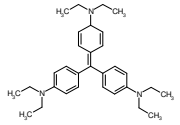
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
067881-18-9	6.724357558	-2.714628777	6.46	5.780341389	18840	4.275
067939-65-5	0.289477947	-16.07050744	2.56	15.23622005	3.162	0.500
068140-48-7	0.55	-2.76	6.31	9.07	2080	3.318
068155-66-8	1.199737182	-1.788687704	4.71	3.104400316	848.1	2.928

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
067881-18-9	P and B	neutral	N	Y	
067939-65-5	Maybe P. Probably not B	neutral	N	Y	
068140-48-7	musk methyl ketone. Great Lakes measurements. Analysable with other hydrocarbons/substituted benzenes by GC-MS	neutral	Y	Y	
068155-66-8	Fragrance? P & B	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
067881-18-9				N			0.5	0.5	0.5
067939-65-5				N	0.5	1	0.5	0.5	0.5
068140-48-7				Y	0.5	0.5	0.5	0.5	0.5
068155-66-8				N			0.5	1	1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
067881-18-9		N	1.55E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
067939-65-5			18.4	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068140-48-7		Y	2.26E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068155-66-8		Y	0.021	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
067881-18-9	67881189	MPV	Neutral Organics
067939-65-5	67939655	MPV	Neutral Organics
068140-48-7	68140487		Neutral Organics
068155-66-8	68155668	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068187-86-0	68187860	
	068608-79-7	68608797	
	068648-87-3	68648873	
	068814-02-8	68814028	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068187-86-0	CCCC(CC(CCC(C(C)CC)CCCC)CC)CCC(CCCC(C)CC(C)CO)CC(C)C	non-halo	9.24E-12	1.2319E-09
068608-79-7	CCCC(C)CC(C)Cc1ccc(cc1)Nc2ccc(cc2)CC(C)CC(C)CCC	Non-halo	2.88E-09	3.84E-07
068648-87-3	c1ccccc1CCCCCCCCCC	Non-halo	2.17E-03	2.89E-01
068814-02-8	CCN(C1C=CC(=C(c3ccc(cc3)N(CC)CC)c2ccc(cc2)N(CC)CC)C=C1)CC	non-halo	2.97E-11	3.95967E-09

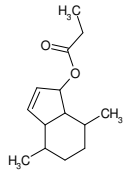
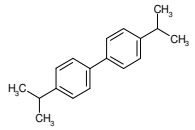
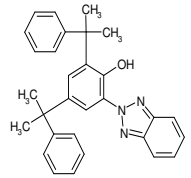
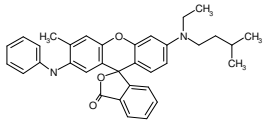
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068187-86-0	2.365531747	0.42567682	15.48	11.66003579	3.162	0.500
068608-79-7	0.05	-2.31	11.95	14.26	3	0.500
068648-87-3	0.62	0.49	6.96	6.47	677	2.831
068814-02-8	0.224033413	-8.347178091	8.18	13.1328907	1552	3.191

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068187-86-0	Probably P (branched and >C32). B questionable	neutral	N	Y	
068608-79-7	Benzenamine, N-phenyl-,(tripropenyl) derivatives. Highly branched hydrocarbon could be P. Probably analysable with hydrocarbons by GC-MS	neutral	N	Y	
068648-87-3	Linear alkylbenzene A-315. Contaminant of Linear alkyl benzene sulfonates. If branched, may be quite persistent. Is amenable to GC-MS analysis	neutral	N	Y	
068814-02-8	Possibly P, maybe B	amine	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068187-86-0				N				0.5	
068608-79-7				N	0.5	0.5	0.5	0.5	10
068648-87-3				N	500	500	500	500	500
068814-02-8				N	0.5	0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068187-86-0			1.54E-15	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068608-79-7		N	3.29E-11	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068648-87-3		Y	1.98E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068814-02-8			0.015	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068187-86-0	68187860	MPV	Phenols
068608-79-7	68608797		Neutral Organics
068648-87-3	68648873		Neutral Organics
068814-02-8	68814028	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	68912-13-0	68912130	
Top 10 non-halogenated	069009-90-1	69009901	
	070321-86-7	70321867	
	070516-41-5	70516415	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
68912-13-0	CCC(=O)OC1C=CC2C(C)CCC(C)C12	Non-halo		
069009-90-1	CC(c1ccc(cc1)c2ccc(cc2)C(C)C)C	Non-halo	7.35E-05	9.80E-03
070321-86-7	Oc(c(cc(c1)C(c(cccc2)c2)(C)C)C(c(cccc3)c3)(C)C)c1N(N=C(C4C=CC5)C=5)N=4	Non-halo	1.63E-14	2.17E-12
070516-41-5	O=C(OC(c(c(Oc1cc(N(CCC(C)C)CC)cc2)cc(c3Nc(cccc4)c4)C)c3)(c12)c5cccc6)c56	Non-halo	1.82E-15	2.43E-13

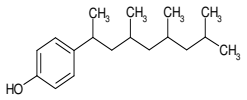
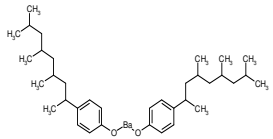
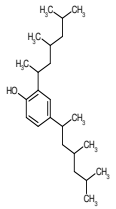
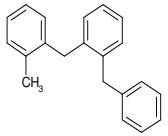
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
68912-13-0	0.06	0.0277	4.28		396.7	2.600
069009-90-1	0.84	-1.20	6.67	7.87	27240	4.435
070321-86-7	0.49	-13.25	7.67	20.92	2755	3.440
070516-41-5	0.05	-12.32	8.72	21.04	288	2.459

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
68912-13-0		neutral	N	Y	
069009-90-1	Substituted biphenyl. Not P but could be B. Analysable with other hydrocarbons.	neutral	N	Y	
070321-86-7	UV absorber used in rubber, polymer industry. Likely analysable by GC-MS after derivatization or possibly by LC-MS (ESI). Similar to 025973-55-1	neutral	N	N	Y
070516-41-5	3-N-Isoamyl-N-ethylamino-6-methyl-7-anilinofluoran. Pigment and dye. Spiro intermediate. May be amenable to GC-MS	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
68912-13-0		Y	Y	N					No Reports
069009-90-1				N			10	10	10
070321-86-7				N	10	10	10	10	10
070516-41-5				N		0.5	1	1	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
68912-13-0	>500K - 1M	N	3.436	Mysid Shrimp 96-hour LC50 (mg/L)	
069009-90-1		Y	7.41E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
070321-86-7		Y	0.058	Fish 96-hour LC_{50} (mg/L)	
070516-41-5		Y	0.000429	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
68912-13-0			Neutral Organics
069009-90-1	69009901		Neutral Organics
070321-86-7	70321867		Neutral Organics
070516-41-5	70516415		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	074499-35-7	74499357	
	078330-15-1	78330151	
	084962-08-3	84962083	
	100404-06-6	100404066	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
074499-35-7	c1c(ccc(c1)C(CC(CC(CC(C)C)C)C)C)O	Non-halo	2.47E-05	3.29E-03
078330-15-1	CC(CC(C)CC(C)CC(C)C)C1=CC=C(O[Ba]OC2=CC=C(C(CC(C)CC(C)CC(C)C)C)C=C2)C=C1	non-halo	3.82E-14	5.09291E-12
084962-08-3	Oc1c(C(C)CC(C)CC(C)C)cc(cc1)C(C)CC(C)CC(C)C	Non-halo	3.15E-07	4.20E-05
100404-06-6	CC1=CC=CC=C1CC2=CC=CC=C2CC3=CC=CC=C3	non-halo	0.00000137	0.000182652

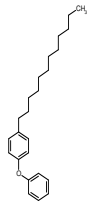
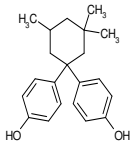
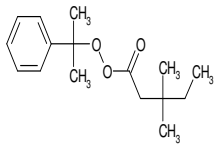
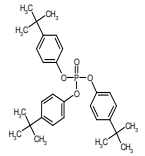
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
074499-35-7	0.19	-3.24	7.17	10.41	37980	4.580
078330-15-1	1.542967641		14.13		3.162	0.500
084962-08-3	0.15	-2.59	10.02	12.61	5	0.667
100404-06-6	6.772416458	-2.714628777	6.59	5.910341389	23480	4.371

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
074499-35-7	Tetrapropenylphenol. Possible EDC. Highly branched - persistent? Some measurements in the Great Lakes region. Like nonyl phenol. Big production. Analysable by GC after derivatization; possibly by LC-MS	phenol	N	N	Y
078330-15-1	P (branched C12 phenol), BCF of phenol 4.58	neutral	N	N	
084962-08-3	DiNonylphenol. Analysable by GC after derivatization; possibly by LC-MS. See also 74499-35-7	phenol	N	N	Y
100404-06-6	P & B, may not be that persistent, rings unsubstituted	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
074499-35-7				N		50	100	100	100
078330-15-1				N	0.5	0.5	1	0.5	
084962-08-3	Y?			N				10	10
100404-06-6				N		0.5	0.5	0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
074499-35-7		Y	2.50E-02	Fish, 96 hr (SAR)	Low
078330-15-1			1.94E-09	Fish, 96 hr (SAR)	
084962-08-3		Y	5.84E-04	Fish, 96 hr (SAR)	
100404-06-6		Y	0.01	Fish, 96 hr (SAR)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
074499-35-7	74499357		Neutral Organics
078330-15-1	78330151	MPV	Surfactants-nonionic + Silanes (alkoxy)
084962-08-3	84962083		Neutral Organics
100404-06-6	100404066	MPV	Phenols + Salicylic Acid

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	119345-02-7	119345027	
	129188-99-4	129188994	
	130097-36-8	130097368	
	000078-33-1	78331	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
119345-02-7	CCCCCCCCCCCCc2ccc(cc2)Oc1ccccc1	Non-halo	1.41E-07	1.88E-05
129188-99-4	CC1CC(C)(C)CC(C2=CC=C(O)C=C2)(C3=CC=C(O)C=C3)C1	non-halo	1.4E-09	1.86651E-07
130097-36-8	O=C(OOC(c1ccccc1)(C)C)CC(CC)(C)C	Non-halo	2.53E-04	3.37E-02
000078-33-1	O=P(Oc(ccc(c1)C(C)(C)C)c1)(Oc(ccc(c2)C(C)(C)C)c2)Oc(ccc(c3)C(C)(C)C)c3	P	2.06E-08	2.74644E-06

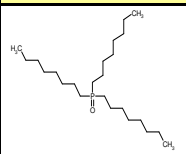
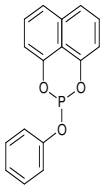
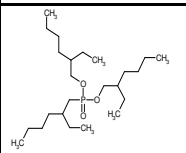
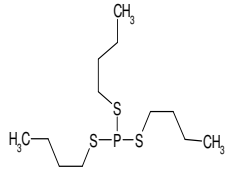
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
119345-02-7	0.41	-0.92	10.00	10.92	3	0.500
129188-99-4	1.459983919	-9.044178502	6.29	11.93989111	13970	4.145
130097-36-8	1.61	-2.97	5.00	7.97	1404	3.147
000078-33-1	8.844744236	-4.552880204	10.43	11.58859282	3.162	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
119345-02-7	Benzene, 1,1'-oxybis-, tetrapropylene derivs. May be persistent if substituents are highly branched. May be analysable by GC-MS with hydrocarbons	neutral	N	Y	
129188-99-4	Possibly P - acylic, branched, Parent - B	phenol	N	N	Y
130097-36-8	Cumyl peroxyneoheptanoate. Polymerization initiator. See also 55794-20-2. May be analysable by GC-MS	neutral	N	Y	
000078-33-1	Might be P - t-butyl. Aryl phosphates do hydrolze. Data in HPV submissions under isobutylated triphenyl phosphate	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
119345-02-7				N		10	10	50	50
129188-99-4				N				0.5	
130097-36-8				N			0.5	0.5	0.5
000078-33-1				N	1	1	1	1	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
119345-02-7		Y	7.24E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	
129188-99-4		Y	0.104	Fish, 96 hr (SAR)	
130097-36-8		Y	0.413	Fish 96-hour LC_{50} (mg/L)	
000078-33-1		Y	0.0168	Fish, 96 hr (SAR)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
119345-02-7	119345027		Neutral Organics
129188-99-4	129188994	MPV	Neutral Organics
130097-36-8	130097368		Benzotriazoles + Phenols
000078-33-1	78331	MPV	Esters + Phenols + Vinyl/Allyl Ketones + Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000078-50-2	78502	
Top 10 non-halogenated	000101-02-0	101020	
	000126-63-6	126636	
	000150-50-5	150505	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000078-50-2	O=P(CCCCCCCC)(CCCCCCCC)CCCCCCCC	p	0.000000378	5.03959E-05
000101-02-0	O(c(cccc1)c1)P(Oc(cccc2)c2)Oc(cccc3)c3	P	7.63E-05	1.02E-02
000126-63-6	O=P(OCC(CCCC)CC)(OCC(CCCC)CC)CC(CCCC)CC	p	0.000000315	4.19965E-05
000150-50-5	CCCCSP(SCCCC)SCCCC	P	1.33E-05	1.77E-03

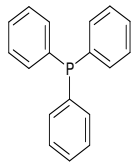
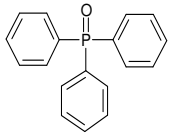
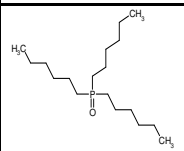
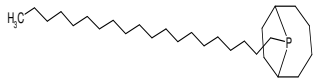
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000078-50-2	4.489625361	-0.30938953	9.76	6.675102142	3.162	0.500
000101-02-0	0.99	-4.66	6.62	11.28	25170	4.401
000126-63-6	1.701141334	-1.708235263	9.51	7.823947874	3.162	0.500
000150-50-5	0.14	-3.03	7.67	10.70	245	2.390

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000078-50-2	Could be quite P - the C-P is not biodegradable	neutral	N	Y	
000101-02-0	HSDB - Chemical intermediate, stabilizer systems for resins, metal scavenger, diluent for epoxy resins. Might oxidize to the triphenyl phosphate since it is used as an antioxidant	neutral	N	Y	
000126-63-6	High Kow - may not be B. C-P bond is persistent	neutral	N	Y	
000150-50-5	Merphos. Organophosphorus herbicide. Used to defoliate cotton. Registration cancelled in 1998 in USA	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000078-50-2				N	0.5	0.5		0.5	
000101-02-0				N	50	50	50	50	50
000126-63-6				N		0.5			
000150-50-5				N		10	10	10	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000078-50-2		N	1.65E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000101-02-0		N	1.11E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000126-63-6		Y	0.004	Fish, 96 hr (SAR)	Low
000150-50-5		N	5.22E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000078-50-2	78502	MPV	Dinitro Amine
000101-02-0	101020		Esters + Phenols
000126-63-6	126636	MPV	Phenols
000150-50-5	150505		Vinyl/Allyl Halides

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 non-halogenated	000603-35-0	603350	
	000791-28-6	791286	
	003084-48-8	3084488	
	013886-99-2	13886992	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000603-35-0	c(P(c(cccc1)c1)c(cccc2)c2)(cccc3)c3	P	1.02E-05	1.36E-03
000791-28-6	O=P(c(cccc1)c1)(c(cccc2)c2)c(cccc3)c3	p	0.000000282	3.75969E-05
003084-48-8	O=P(CCCCCC)(CCCCCC)CCCCCC	p	0.0000302	0.004026336
013886-99-2	CCCCCCCCCCCCCCCCCCCCP1C2CCCCC1CC2	P	1.57E-08	2.09E-06

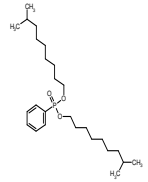
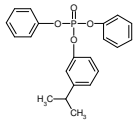
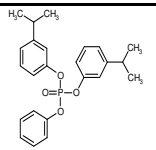
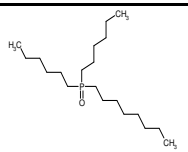
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000603-35-0	1.83	-6.03	5.02	11.05	4801	3.681331706
000791-28-6	21.94374403	-7.667585032	3.1	7.373297643	30.14	1.479
003084-48-8	6.382225166	-1.046148095	6.81	4.461860707	1113	3.046
013886-99-2	0.00	1.11	12.93	11.82	1	-0.301

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000603-35-0	Triphenylphosphine	neutral	N	Y	
000791-28-6	Might be very stable - three C-P bonds	neutral	N	Y	
003084-48-8	C-P stable = P, Could be B	neutral	N	Y	
013886-99-2	Eicosyl Phobane. Catalyst ligand in hydroformylation chemistry such as in fatty alcohol manufacture from olefins. May be analysable with other hydrocarbons/substituted benzenes by GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000603-35-0				N	1	10	10	10	10
000791-28-6				N		0.5	0.5	0.5	
003084-48-8				N				0.5	
013886-99-2				N	0.5	1	0.5	10	1

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000603-35-0		N	1.37E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
000791-28-6		Y	2.509	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
003084-48-8		Y	6.28E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
013886-99-2		N	1.97E-12	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000603-35-0	603350		Halopyridine
000791-28-6	791286	MPV	Neutral Organics
003084-48-8	3084488	MPV	Phenols
013886-99-2	13886992		Thiols(mercaptans)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	025550-98-5	25550985	
	028108-99-8	28108998	
	028109-00-4	28109004	
	031160-64-2	31160642	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
025550-98-5	O=P(c1ccccc1)(OCCCCCCCCC(C)C)OCCCCCCCCC(C)C	P	2.19E-08	2.92E-06
028108-99-8	CC(C)(C)c3ccc(OP(=O)(Oc1ccccc1)Oc2ccccc2)cc3	P	2.61E-08	3.48E-06
028109-00-4	O=P(Oc1cccc(c1)C(C)C)(Oc2cc(ccc2)C(C)C)Oc3ccccc3	P	2.06E-08	2.74644E-06
031160-64-2	O=P(CCCCCC)(CCCCCCCC)CCCCCC	p	0.00000531	0.000707942

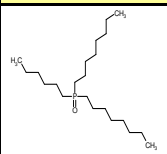
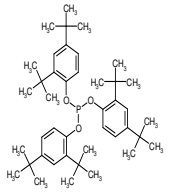
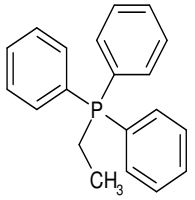
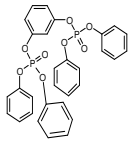
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
025550-98-5	0.15	-3.67	9.32	12.99	3	0.500
028108-99-8	0.00	-5.38	6.61	11.99	4	0.558
028109-00-4	5.07116183	-5.209593829	7.61	9.42530644	1551	3.191
031160-64-2	5.595906802	-0.79973905	7.8	5.205451662	165.9	2.220

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
025550-98-5	Diisodecyl Phenyl Phosphite. DSL assessment predicts persistent. Hydrolysis important. Analysable by GC-MS like triaryl/alkyl phosphates. Phosphite degradation product may be analysable by LC-MS.	neutral	N	Y	
028108-99-8	Phosphate flame retardant phosphate. Isopropyl diphenyl phosphate. Limited environmental measurements in the Great Lakes region	neutral	N	Y	
028109-00-4	Check triaryl phosphates - could be P & B. P questionable	neutral	N	Y	
031160-64-2	P (stable C-P bond). Could be B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
025550-98-5		aryl phosphite	Y?	N					
028108-99-8				N	0.5	0.5	1	10	1
028109-00-4				N		0.5	0.5	1	0.5
031160-64-2				N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
025550-98-5		N	8.00E-03	Fish, 96 hr (SAR)	Low
028108-99-8		Y	0.034	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
028109-00-4		Y	0.04	Fish, 96 hr (SAR)	Marginal
031160-64-2		Y	3.97E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
025550-98-5	25550985		Esters + Esters (phosphate)
028108-99-8	28108998		Esters + Esters (phosphate)
028109-00-4	28109004	MPV	Neutral Organics
031160-64-2	31160642	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	031160-66-4	31160664	
	031570-04-4	31570044	
	035835-94-0	35835940	
	057583-54-7	57583547	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
031160-66-4	O=P(CCCCCC)(CCCCCCCC)CCCCCCCC	p	0.00000134	0.000178652
031570-04-4	O(c(c(cc(c1)C(C)(C)C)C(C)(C)C)c1)P(Oc(c(cc(c2)C(C)(C)C)C(C)(C)C)c2)Oc(c(cc(c3)C(C)(C)C)C(C)(C)C)c3	P	4.74E-14	6.32E-12
035835-94-0	CCP(c2ccccc2)(c3ccccc3)(c1ccccc1)OC(=O)C	p	2.92E-08	3.89301E-06
057583-54-7	c1(OP(=O)(Oc4ccccc4)Oc2cc(OP(=O)(Oc5ccccc5)Oc3ccccc3)ccc2)ccccc1	p	2.06E-08	2.74644E-06

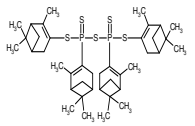
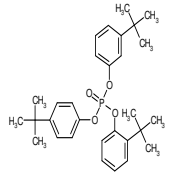
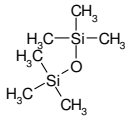
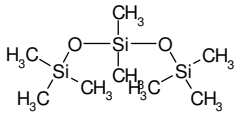
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
031160-66-4	4.982093075	-0.554150072	8.78	5.939862684	7.486	0.874
031570-04-4	0.45	-2.18	18.08	20.26	3	0.500
035835-94-0	18.35566133	-8.143058108	-1.36	3.38877072	3.162	0.500
057583-54-7	6.067555319	-10.92022345	7.41	14.93593606	2956	3.471

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
031160-66-4	P (stable C-P bond) could be B	neutral	N	Y	
031570-04-4	Phosphate flame retardant phosphate. Tri(t-butylphenyl) phosphate. Limited environmental measurements in the Great Lakes region	neutral	Y	Y	
035835-94-0	P? (C-P bond stable). Ethyltriphenylphosphonium acetate	neutral	N	Y	
057583-54-7	Might hydrolyze. High Kow and B	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
031160-66-4				N				0.5	
031570-04-4				N	10	10	10	50	50
035835-94-0				N	0.5	0.5	0.5	0.5	0.5
057583-54-7				N					0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
031160-66-4		N	2.57E-07	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
031570-04-4		N	1.10E-18	Mysid Shrimp 96-hour LC_{50} (mg/L)	
035835-94-0		Y	0.154	Mysid Shrimp 96-hour LC_{50} (mg/L)	
057583-54-7		Y	0.071	Fish, 96 hr (SAR)	Marginal

CASRN	CASRN (without hyphens)	category	EcoSAR class
031160-66-4	31160664	MPV	Neutral Organics
031570-04-4	31570044		Esters
035835-94-0	35835940	MPV	Neutral Organics
057583-54-7	57583547	MPV	Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068400-79-3	68400793	
	068937-40-6	68937406	
	000107-46-0	107460	
	000107-51-7	107517	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068400-79-3	CC7=C(SP(=S)(SP(=S)(SC1=C(C)C2CC(C1)C2(C)C)C3=C(C)C4CC(C3)C4(C)C)C5=C(C)C6CC(C5)C6(C)C)CC8CC7C8(C)C	P	2.06E-08	2.75E-06
068937-40-6	O=P(Oc1ccc(cc1)C(C)(C)C)(Oc2ccc(cc2)C(C)(C)C)Oc3ccc(cc3)C(C)(C)C	P	2.06E-08	2.75E-06
000107-46-0	C[Si](C)(C)O[Si](C)(C)C	Si	3.91E+01	5.21E+03
000107-51-7	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	3.49E+00	4.65E+02

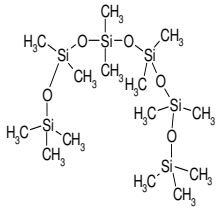
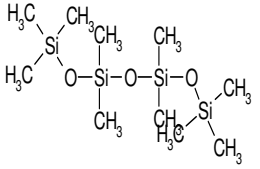
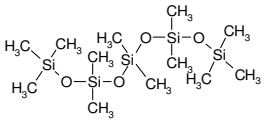
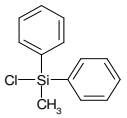
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068400-79-3	0.01	11.61	16.95	5.34	1	-0.301
068937-40-6	0.74	-5.55	10.43	15.98	3	0.500
000107-46-0	11.92	1.09	4.76	3.67	342	2.534
000107-51-7	8.94	1.23	5.35	4.12	991	2.996

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068400-79-3	bis(2,6,6-trimethylbicyclo[3.1.1]hept-2-enyl) bis(2,6,6-trimethylbicyclo[3.1.1]hept-2-enyl)thiodiphosphonate. Possible use as flame retardant? May not be amanable to GC-MS due to number of thio linkages	neutral	N	Y?	
068937-40-6	Phosphate ester flame retardant. May be persistent (t-butyl group on ring) - hydrolysis important? Limited measurements in the Great Lakes region. See also 31570-04-4.	neutral	Y	Y	
000107-46-0	very volatile but probably amenable to GC analysis	neutral	N	Y	
000107-51-7	very volatile but probably amenable to GC analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068400-79-3				N	10	1	1	10	1
068937-40-6				N	10	1	1	1	10
000107-46-0				N	10	10	10	50	50
000107-51-7				N	0.5	0.5	1	1	10

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068400-79-3		N	3.35E-17	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068937-40-6		N	1.68E-02	Fish, 96 hr (SAR)	Marginal
000107-46-0		N	6.20E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000107-51-7		N	1.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
068400-79-3	68400793		Neutral Organics
068937-40-6	68937406		Phenols
000107-46-0	107460		Phenols
000107-51-7	107517		Neutral organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000107-52-8	107528	
	000141-62-8	141628	
Top 10 siloxanes	000141-63-9	141639	
	000144-79-6	144796	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000107-52-8	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	3.46E-02	4.61E+00
000141-62-8	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	4.86E-01	6.48E+01
000141-63-9	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	7.04E-02	9.39E+00
000144-79-6	Cl[Si](c1ccccc1)(c2ccccc2)C	Si	1.33E-03	1.77E-01

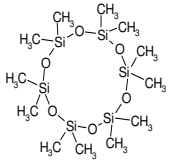
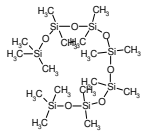
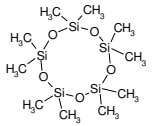
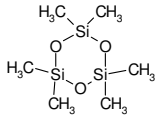
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000107-52-8	5.11	0.65	7.10	6.46	24100	4.382
000141-62-8	7.15	1.37	5.93	4.56	2871	3.458
000141-63-9	5.96	1.51	6.52	5.01	8318	3.920
000144-79-6	2.64	-2.00	5.29	7.29	2381	3.377

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000107-52-8	Tetradecamethylhexasiloxane. May have similar properties to D6 cyclic siloxane which has been analysed by GC-MS	neutral	N	Y	
000141-62-8	very volatile but probably amenable to GC analysis	neutral	N	Y	
000141-63-9	Dodecamethylpentasiloxane. May have similar properties to D5 cyclic siloxane which has been analysed by GC-MS	neutral	N	Y	
000144-79-6	chlorosiloxane could hydrolyse	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000107-52-8				N					0.5
000141-62-8				N	0.5	0.5	0.5	0.5	1
000141-63-9				N	0.5	0.5	0.5	0.5	0.5
000144-79-6		silanol	Y	N	0.5	10	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000107-52-8		N	1.75E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000141-62-8		N	4.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000141-63-9		N	8.23E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000144-79-6		N	4.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low-moderate

CASRN	CASRN (without hyphens)	category	EcoSAR class
000107-52-8	107528		Esters
000141-62-8	141628		anilines
000141-63-9	141639		Neutral Organics
000144-79-6	144796		amine

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 siloxanes	000540-97-6	540976	
Top 10 siloxanes	000541-01-5	541015	
Top 10 siloxanes	000541-02-6	541026	
	000541-05-9	541059	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000540-97-6	C[Si]1(O[Si](O[Si](O[Si](O[Si](C)(C)O[Si](O1)(C)C)(C)C)(C)C)(C)C)C	Si	3.55E-02	4.73E+00
000541-01-5	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	9.23E-03	1.23E+00
000541-02-6	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	Si	2.18E-01	2.91E+01
000541-05-9	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O1	Si	3.29E+00	4.39E+02

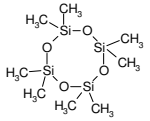
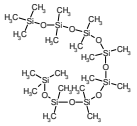
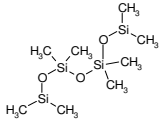
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
000540-97-6	5.96	0.83	6.33	5.50	14890	4.173
000541-01-5	4.47	0.78	7.69	6.91	34360	4.536
000541-02-6	7.15	0.69	5.71	5.02	2014	3.304
000541-05-9	11.92	0.41	4.47	4.06	549	2.739

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000540-97-6	DMethodology under development; some environmental measurements in the Great Lakes	neutral	Y	Y	
000541-01-5	Methodology under development; some environmental measurements	neutral	Y	Y	
000541-02-6	D5. Methodology under development; some environmental measurements in the Great Lakes	neutral	Y	Y	
000541-05-9	D3. Methodology under development; some environmental measurements	neutral	Y	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000540-97-6				N	0.5	10	10	10	50
000541-01-5				N					0.5
000541-02-6				N	50	50	50	100	500
000541-05-9				N	1	10	1	1	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000540-97-6		N	3.68E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000541-01-5		N	3.60E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
000541-02-6		N	8.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000541-05-9		N	3.90E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
000540-97-6	540976		Hydrazines
000541-01-5	541015		Esters + Esters (phosphate)
000541-02-6	541026		Esters + Phenols
000541-05-9	541059		Aliphatic amine + Vinyl/Allyl Halides + Vinyl/Allyl Ethers

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	000546-56-5	546565	
Top 10 siloxanes	000556-67-2	556672	
Top 10 siloxanes	000556-69-4	556694	
	001000-05-1	1000051	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
000546-56-5	O1[Si](O[Si](O[Si](O[Si]1(c2ccccc2)c3ccccc3)(c4ccccc4)c5ccccc5)(c6ccccc6)c7ccccc7)(c8ccccc8)c9ccccc9	Si	5.91E-18	7.88E-16
000556-67-2	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	Si	1.18E+00	1.57E+02
000556-69-4	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	1.04E-02	1.39E+00
001000-05-1	[Si](O[Si](O[Si](O[Si](C)C)(C)C)(C)C)(C)C	Si	1.26E-01	1.68E+01

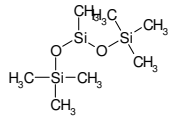
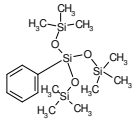
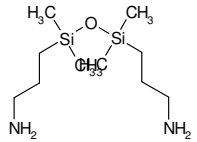
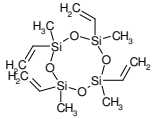
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
000546-56-5	0.69	-9.13	14.82	23.95	3	0.500
000556-67-2	8.94	0.55	5.09	4.54	1687	3.227
000556-69-4	3.97	0.92	8.28	7.36	7096	3.851
001000-05-1	8.94	1.09	4.84	3.75	1061	3.026

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
000546-56-5	May be analysable with similar methodology as cyclic siloxanes	neutral	N	Y?	
000556-67-2	D4. Methodology under development; some environmental measurements in the Great Lakes	neutral	Y	Y	
000556-69-4	Methodology under development; some environmental measurements	neutral	N	Y	
001000-05-1	May be analysable with similar methodology as cyclic siloxanes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
000546-56-5				N	0.5	0.5	0.5	0.5	0.5
000556-67-2				N	500	500	500	500	500
000556-69-4				N					0.5
001000-05-1				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
000546-56-5		N	1.60E-14	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000556-67-2		N	8.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	
000556-69-4		N	9.74E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
001000-05-1		N	1.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
000546-56-5	546565		Neutral Organics
000556-67-2	556672		Esters
000556-69-4	556694		Vinyl/Allyl Halides
001000-05-1	1000051		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	001873-88-7	1873887	
Top 10 siloxanes	002116-84-9	2116849	
	002469-55-8	2469558	
Top 10 siloxanes	002554-06-5	2554065	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
001873-88-7	C[Si](O[Si](C)(C)C)O[Si](C)(C)C	Si	2.70E+00	3.60E+02
002116-84-9	C[Si](O[Si](c1ccccc1)(O[Si](C)(C)C)O[Si](C)(C)C)(C)C	Si	2.35E-03	3.13E-01
002469-55-8	[Si](O[Si](C)(C)CCCN)(C)(C)CCCN	Si	2.54E-03	3.39E-01
002554-06-5	C=C[Si]1(O[Si](O[Si](O[Si](O1)(C=C)C)(C=C)C)(C=C)C)C	Si	1.07E-01	1.43E+01

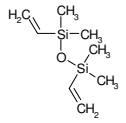
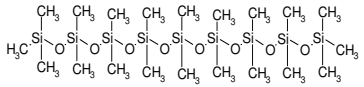
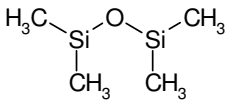
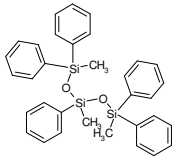
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
001873-88-7	10.21	0.09	4.80	4.71	991	2.996
002116-84-9	3.24	0.16	7.15	6.99	40260	4.605
002469-55-8	0.15	-7.39	3.78	11.17	164	2.214
002554-06-5	0.10	0.56	6.51	5.95	20410	4.310

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
001873-88-7	very volatile but probably amenable to GC analysis	neutral	N	Y	
002116-84-9	May be analysable with similar methodology as cyclic siloxanes. ' P & B Check trialkoxysiloxanes - hydrolysis?	neutral	N	Y	
002469-55-8	1,3-Bis(aminopropyl)tetramethyldisiloxane.flexibilizing hardener for epoxies, endcapper for aminopropyl terminated silicones. May not be analysable with other cyclic and linear siloxanes due to NH2 groups	neutral	N	N	
002554-06-5	2,4,6,8-Tetravinyl-2,4,6,8-tetramethylcyclotetrasiloxane. Similar to D4 in terms of phys-chem properties. Should be amenable to GC-MS analysis	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
001873-88-7				N	0.5	0.5	1	1	10
002116-84-9				N	0.5	0.5	1	0.5	
002469-55-8				N		0.5			0.5
002554-06-5				N	0.5	0.5	0.5	0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
001873-88-7		N	1.50E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
002116-84-9		N	2.91E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
002469-55-8		Y	3.687	Fish 96-hour LC_{50} (mg/L)	Low
002554-06-5		N	1.70E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
001873-88-7	1873887		Acid Chloride/Halide
002116-84-9	2116849		Neutral Organics
002469-55-8	2469558		Neutral Organics
002554-06-5	2554065		Methacrylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	002627-95-4	2627954	
	002652-13-3	2652133	
	003277-26-7	3277267	
	003390-61-2	3390612	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
002627-95-4	C=C[Si](O[Si](C=C)(C)C)(C)C	Si	4.49E+02	5.99E+04
002652-13-3	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Si	1.31E-03	1.75E-01
003277-26-7	C[Si](C)O[Si](C)(C)C	Si	1.21E+02	1.61E+04
003390-61-2	C[Si](c1ccccc1)(O[Si](c2ccccc2)(c3ccccc3)C)O[Si](c4ccccc4)(c5ccccc5)C	Si	2.05E-12	2.73E-10

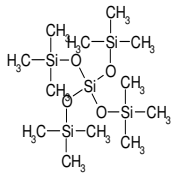
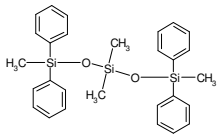
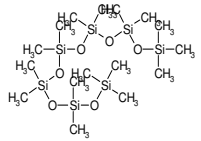
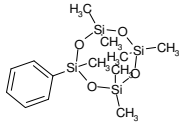
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
002627-95-4	0.19	1.10	5.47	4.37	3257	3.513
002652-13-3	3.57	1.06	8.86	7.80	1069	3.029
003277-26-7	14.30	-0.04	4.21	4.25	351	2.545
003390-61-2	1.05	-4.82	11.43	16.25	3	0.500

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
002627-95-4	May be similar to D3 in phys-chem properties. Should be amenable to GC-MS analysis	neutral	N	Y?	
002652-13-3	Hexacosamethylcyclotridecasiloxane. Semivolatile. May be amenable to GC-MS analysis	neutral	N	Y	
003277-26-7	Very volatile linear siloxane.	neutral	N	N	
003390-61-2	rimethylpentaphenyltrisiloxane. Silicone diffusion pump fluid. Very low VP compared to most siloxanes. May nevertheless be amenable to GC-MS	neutral	N	Y?	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
002627-95-4				N	0.5	0.5	1	1	10
002652-13-3				N	0.5				
003277-26-7				N	0.5	0.5	0.5	0.5	1
003390-61-2				N	0.5	0.5		0.5	0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
002627-95-4		N	1.83E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
002652-13-3		N	1.94E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
003277-26-7		N	5.50E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
003390-61-2		N	1.91E-10	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
002627-95-4	2627954		Methacrylates
002652-13-3	2652133		Neutral Organics
003277-26-7	3277267		Neutral Organics
003390-61-2	3390612		Methacrylates

Priorities	CASRN	CASRN (without hyphens)	Molstructure
Top 10 siloxanes	003555-47-3	3555473	
	003982-82-9	3982829	
	009006-65-9	9006659	
Top 10 siloxanes	010448-09-6	10448096	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
003555-47-3	[Si](O[Si](O[Si](C)(C)C)(O[Si](C)(C)C)O[Si](C)(C)C)(C)(C)C	Si	1.51E-01	2.01E+01
003982-82-9	C[Si](O[Si](c1ccccc1)(c2ccccc2)C)(O[Si](c3ccccc3)(c4ccccc4)C)C	Si	5.86E-10	7.81E-08
009006-65-9	C[Si](O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C)(C)O[Si](C)(C)C	Si	9.23E-03	1.23E+00
010448-09-6	C[Si]1(C2=CC=CC=C2)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	Si	2.56E-03	3.41E-01

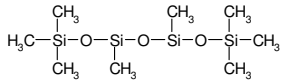
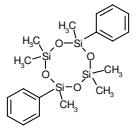
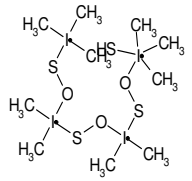
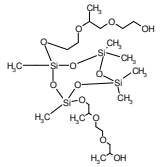
CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
003555-47-3	5.96	1.51	6.52	5.01	20860	4.319
003982-82-9	1.27	-3.61	10.21	13.82	3	0.500
009006-65-9	4.47	1.78	7.69	5.91	34360	4.536
010448-09-6	3.57	-0.66	6.30	6.96	14260	4.154

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
003555-47-3	Tetrakis(trimethylsilyloxy)silane or Trisiloxane. Used as a pesticide adjuvant. May be analysable by GC-MS although highly volatile similar to D6.	neutral	N	Y	
003982-82-9	1,1,5,5-Tetraphenyl-1,3,3,5-tetramethyltrisiloxane. Use in diffusion pump oil. See also 3390-61-2	neutral	N	Y	
009006-65-9	dimethicone. Known as "silicone fluid". Should be analysable by GC-MS similar to cyclic siloxanes	neutral	N	Y	
010448-09-6	heptamethyl-phenyl-cyclotetrasiloxane. Should be analysable by GC-MS similar to cyclic siloxanes	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
003555-47-3				N					
003982-82-9				N	0.5	0.5	0.5	0.5	0.5
009006-65-9				N					
010448-09-6				N					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
003555-47-3		N	1.84E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	
003982-82-9		N	5.66E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	
009006-65-9		N	8.80E-06	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
010448-09-6		N	3.23E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
003555-47-3	3555473		Methacrylates
003982-82-9	3982829		Acrylates
009006-65-9	9006659		Neutral Organics
010448-09-6	10448096		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	016066-09-4	16066094	
	033204-76-1	33204761	
	063148-62-9	63148629	
	064365-23-7	64365237	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
016066-09-4	[Si](O[Si](O[Si](O[Si](C)(C)C)C)C)(C)(C)C	Si	1.56E+00	2.08E+02
033204-76-1	[Si]1(C)(C)O[Si](C)(c3ccccc3)O[Si](C)(C)O[Si](C)(c2ccccc2)O1	Si	8.37E-06	1.12E-03
063148-62-9	Si(C)(C)(C)OSi(C)(C)OSi(C)(C)OSi(C)(C)(C)	Si	4.86E-01	6.48E+01
064365-23-7	OC(C)COCCOC(C)COCCOSi(C)(C)OSi(C)(C)OSi(C)(C)OSi(C)(C)OCC(C)OCCOC(C)COCCO	Si	2.39E-16	3.19E-14

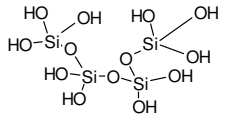
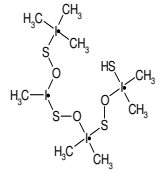
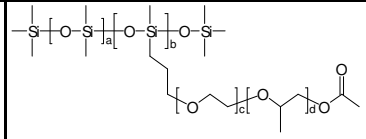
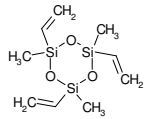
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
016066-09-4	8.94	0.09	4.84	4.75	1061	3.026
033204-76-1	2.23	-1.87	7.52	9.39	12490	4.097
063148-62-9	7.15	1.37	5.93	4.56	2871	3.458
064365-23-7	0.08	-16.89	1.90	18.79	6	0.765

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
016066-09-4	1,1,1,3,5,7,7,7-octamethyl-tetrasiloxane. Should be analysable by GC-MS similar to cyclic siloxanes	neutral	N	Y	
033204-76-1	2,6-cis-Diphenylhexamethyl cyclotetrasiloxane. High temperature bearing grease. Very low VP compared to most siloxanes - simila rto pump diffusion oils. Should be analysable by GC-MS	neutral	N	Y	
063148-62-9	Silcone fluid similar to 9006-65-9. Used in personal care products with excellent spreading and unique volatility characteristics. Antifoaming agent. Should be amenable to GC-MS	neutral	N	Y	
064365-23-7	Used in personal care products. Should be amenable to GC-MS	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
016066-09-4				N	0.5	0.5			
033204-76-1				N					
063148-62-9				N	0.5		10	0.01	0.5
064365-23-7				N					0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
016066-09-4		N	1.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
033204-76-1		N	1.13E-05	Mysid Shrimp 96-hour LC_{50} (mg/L)	
063148-62-9		N	8.13E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
064365-23-7		Y	16.518	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
016066-09-4	16066094		Neutral Organics
033204-76-1	33204761		Neutral Organics
063148-62-9	63148629		amine
064365-23-7	64365237		Phenols

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	067762-90-7	67762907	
	068037-59-2	68037592	
	068037-64-9	68037649	
	068082-23-5	68082235	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
067762-90-7	Si(C)(C)(C)OSi(C)(C)OSi(C)(C)OSi(C)(C)OSi(O)(O)OSi(O)(O)OSi(O)(O)OSi(O)(O)O	Si	3.83E-19	5.11E-17
068037-59-2	Si(C)(C)OSi(C)(C)OSi(C)OSi(C)(C)(C)	Si	1.26E-01	1.68E+01
068037-64-9	No structure – SRC provided structure	Si		
068082-23-5	C=C[Si]1(O[Si](O[Si](O1)(C=C)C)(C=C)C)C	Si	1.21E+00	1.61E+02

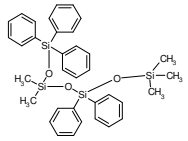
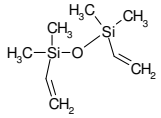
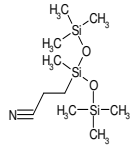
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
067762-90-7	0.33	-30.84	-8.92	21.92	3	0.500
068037-59-2	8.94	1.09	4.84	3.75	1061	3.026
068037-64-9						
068082-23-5	0.13	0.42	5.53	5.11	3621	3.559

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
067762-90-7	Nonvolatile. Amorphous fused silica. Analytical method uncertain.	neutral	N	N	
068037-59-2	dimethyl, methylhydrogen siloxane. Used as leak sealant and in adhesive applications. Similar VP to cyclic siloxanes - should be amenable to GC-MS analysis	neutral	N	Y	
068037-64-9	Siloxanes and Silicones, di-Me, Me hydrogen, reaction products with polyethylene-polypropylene glycol monoacetate allylether	polymer	N	N	
068082-23-5	May be similar to D3 in properties. See also 2627-95-4	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
067762-90-7				N	1	1	10	10	10
068037-59-2				N					
068037-64-9				N					
068082-23-5				N					0.5

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
067762-90-7		N	4.73E+15	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
068037-59-2		N	1.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068037-64-9		N	NA	Fish 96-hour LC_{50} (mg/L)	
068082-23-5		N	2.00E-03	Mysid Shrimp 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
067762-90-7	67762907		Neutral Organics
068037-59-2	68037592		Peroxy Acids
068037-64-9	68037649		Thiols(mercaptans)
068082-23-5	68082235		Peroxy Acids

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	068083-14-7	68083147	
	068478-92-2	68478922	
	068938-51-2	68938512	
	068957-05-1	68957051	No structure Chlorinated phenyl methyl polysiloxane

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
068083-14-7	Si(C)(C)(C)OSi(c1ccccc1)(c1ccccc1)OSi(C)(C)OSi(c1ccccc1)(c1ccccc1)(c1ccccc1)	Si	3.64E-13	4.85E-11
068478-92-2	C=CSi(C)(C)OSi(S)(S)C=C	Si	6.72E-02	8.96E+00
068938-51-2	C[Si](C)(C)O[Si](CCC#N)(C)O[Si](C)(C)C	Si	1.55E-02	2.07E+00
068957-05-1	No structure	Si		

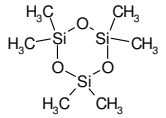
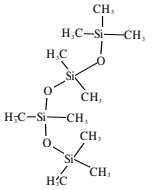
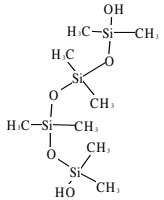
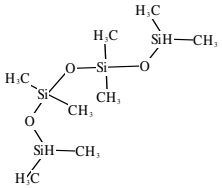
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
068083-14-7	1.02	-4.68	12.02	16.70	3	0.500
068478-92-2	0.19	-1.83	4.38	6.21	468	2.670
068938-51-2	7.70	-2.03	4.86	6.89	1103	3.043
068957-05-1						

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
068083-14-7	Polydimethyldiphenyl Siloxane Copolymer. Use in applications where Dimethyl siloxanes will not remain stable e.g. heat exchangers, dielectric coolants, and base oils	neutral	N	Y	
068478-92-2	May be similar to D3 in properties. See also 2627-95-4	neutral	N	Y	
068938-51-2	(Cyanopropyl)-Methyl. (48-50%)-Methylphenyl-. Siloxane Copolymer. May be amenable to GC-MS similar to other methyl siloxanes	neutral	N	Y	
068957-05-1	Tetrachlorophenylsilsesquioxane-Dimethylsiloxane. A thermal Silicone Fluids for Mechanical and Heat Transfer Applications similar to other siloxanes. Highly stable so likely amenable to GC-MS analysis	polymer	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
068083-14-7				N			0.5		
068478-92-2				N		0.5		0.5	0.5
068938-51-2				N					
068957-05-1				N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
068083-14-7		N	3.96E-11	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068478-92-2		Y	5.00E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Marginal
068938-51-2		N	1.60E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
068957-05-1		N	NA	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
068083-14-7	68083147		Dinitrobenzenes
068478-92-2	68478922		Neutral Organics
068938-51-2	68938512		Neutral Organics
068957-05-1	68957051		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	069430-24-6	69430246	
	069430-47-3	69430473	
	070131-67-8	70131678	
	070900-21-9	70900219	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
069430-24-6	C[Si]1(O[Si](O[Si](O1)(C)C)(C)C)C	Si	3.29E+00	4.39E+02
069430-47-3	Si(C)(C)(C)OSi(C)(C)OSi(C)(C)OSi(C)(C)(C)	Si	4.86E-01	6.48E+01
070131-67-8	Si(C)(C)(O)OSi(C)(C)OSi(C)(C)OSi(C)(C)(O)	Si	3.53E-05	4.71E-03
070900-21-9	Si(C)(C)OSi(C)(C)OSi(C)(C)OSi(C)(C)	Si	1.26E-01	1.68E+01

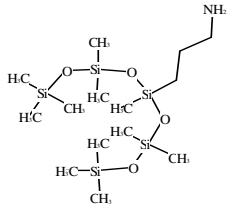
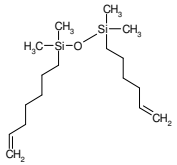
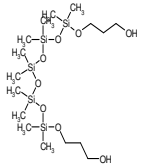
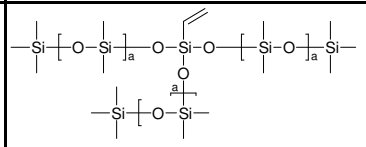
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
069430-24-6	11.92	0.41	4.47	4.06	549	2.739
069430-47-3	7.15	1.37	5.93	4.56	2871	3.458
070131-67-8	1.32	-5.91	2.43	8.34	15	1.169
070900-21-9	8.94	1.09	4.84	3.75	1061	3.026

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
069430-24-6	Cyclomethicone. Seems to be identical to 541-05-9. Used in some personal care products	neutral	N	Y	
069430-47-3	Linear methylsiloxane - similar properties to other methyl siloxanes. Should be amenable to GC-MS analysis	neutral	N	Y	
070131-67-8	Silanol or "hydroxy terminated" siloxane. Low VP. May not be amenable to GC analysis due to high polarity of OH moiety	neutral	N	Y?	
070900-21-9	Hydride terminated Polydimethylsiloxane. Similar VP to other linear methyl siloxanes so should be amenable to GC-MS analysis	neutral	N	Y	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
069430-24-6				N				0.5	0.5
069430-47-3				N					
070131-67-8				N				0.5	
070900-21-9				N				0.5	

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
069430-24-6		N	3.90E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	
069430-47-3		N	8.13E-04	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
070131-67-8		N	1.95E+01	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
070900-21-9		N	1.70E-02	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low

CASRN	CASRN (without hyphens)	category	EcoSAR class
069430-24-6	69430246		Neutral Organics
069430-47-3	69430473		Esters + Esters (phosphate)
070131-67-8	70131678		Neutral Organics
070900-21-9	70900219		Esters + Esters (phosphate)

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	099363-37-8	99363378	
	104360-37-4	104360374	
	104780-66-7	104780667	
	126581-51-9	126581519	

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
099363-37-8	C[Si](O[Si](O[Si](O[Si](O[Si](C)(C)C)(C)C)(CCCN)C)(C)C)(C)C	Si	1.41E-02	1.88E+00
104360-37-4	C=CCCCCC[Si](C)(C)OSi(C)(C)CCCCC=C	Si	1.62E-03	2.16E-01
104780-66-7	OCCCO[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)OCCCO	Si	4.10E-09	5.47E-07
126581-51-9	C[Si](O[Si](O[Si](O[Si](C)(C)C)(CCCOCCOC(COC(=O)C)C)C)(C)C)(C)C	Si	4.60E-06	6.13E-04

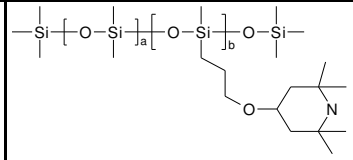
CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF
099363-37-8	3.57	-2.23	6.03	8.26	8769	3.943
104360-37-4	0.12	1.19	9.89	8.70	3	0.500
104780-66-7	0.34	-6.15	3.45	9.60	90	1.954
126581-51-9	2.9 h	-4.50	6.32	10.82	14791.08	4.170

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
099363-37-8	Aminopropylmethylsiloxane-dimethylsiloxane copolymer; polymer modifier; mold release agent; lubricant. No structure – SRC provided SMILE	amine	N	Y?	
104360-37-4	Long chain substituents give lower VP. Should be amenable to GC-MS analysis	neutral	N	Y	
104780-66-7	Carbinol (Hydroxy) Functional Siloxanes - used as reactive additive in polyurethanes, epoxies, polyesters and phenolics. With reactive OH moiety may not be amenable to GC-MS analysis. Low VP. May be amenable to LC-MS	neutral	N	N	
126581-51-9	Vinylphenylmethyl Terminated Dimethyl Siloxanes. No structure – SRC provided structure and SMILE	polymer	N	N	

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
099363-37-8				N			0.5	0.5	0.5
104360-37-4				N			0.5	0.5	0.5
104780-66-7	Y?			N					0.5
126581-51-9				N		0.5			

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
099363-37-8		Y	9.83E-08	Mysid Shrimp 96-hour LC_{50} (mg/L)	
104360-37-4		N	9.17E-09	Mysid Shrimp 96-hour LC_{50} (mg/L)	Low
104780-66-7		Y	2.324	Fish 96-hour LC_{50} (mg/L)	
126581-51-9		N	1.62E+01	Fish 96-hour LC_{50} (mg/L)	

CASRN	CASRN (without hyphens)	category	EcoSAR class
099363-37-8	99363378		Neutral Organics
104360-37-4	104360374		Neutral Organics
104780-66-7	104780667		Neutral Organics
126581-51-9	126581519		Neutral Organics

Priorities	CASRN	CASRN (without hyphens)	Molstructure
	146832-03-3	146832033	No structure
	182635-99-0	182635990	

[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.

51 [b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).

0 Footnotes 610

CASRN	Smiles	Class	VP est. (mmHg)	VP est. (Pa)
146832-03-3	C([Si](O[Si](O[Si](O[Si](CCCCCCCCCCCCCCCC)(C)C)(C)C)(C)C)(C)C)(C)C)CCCCCCCCCCC	Si	1.28E-11	
182635-99-0	C[Si](O[Si](O[Si](O[Si](C)(C)C)(C)CCCOC1CC(C)(C)NC(C)(C)C1)(C)C)(C)C	Si	1.23E-06	1.64E-04

[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.

[b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).

Footnotes

Cl	116	19.02%	
F	181	29.67%	
Br	80	13.11%	
Non-halo	165	27.05%	
Si	48	7.87%	

CASRN	Atmospheric Oxidation $t_{1/2}$	$LogK_{aw}$	$LogK_{ow}$	$LogK_{oa}$	BCF	logBCF
146832-03-3	3.401 h	4.71	19.29	14.58	3.16227766	0.5
182635-99-0	1.31	-3.46	7.72	11.18	6574	
					604	

[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.

[b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).

Footnotes

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
146832-03-3	Siloxanes and Silicones, di-Me, mono(3-((2-methyl-1-oxo-2-propenyl)oxy)propyl group)-terminated, polymers. No structure – SRC provided structure and SMILE	polymer	N	N	
182635-99-0	Siloxanes and silicones, methyl hydrogen, reaction products with 2,2,6,6-tetramethyl-4-(2-propenyloxy)piperidine. No structure – SRC provided structure and SMILE	amine	N	N	
[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.	N=	0.83442623	509	167	0
[b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).	Y=	0.16557377	101	404	70
Footnotes	total		610	610	78
	Maybe		0	39	8

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
146832-03-3				N			0.5		
182635-99-0				N					0.5
[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.	0	0	0						0.709447415
[b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).	43	5	185						
Footnotes	68	199	193	609					
	24	0	4						

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
146832-03-3		N	NA	Mysid Shrimp 96-hour LC_{50} (mg/L)	
182635-99-0		N	7.00E-03	Fish 96-hour LC_{50} (mg/L)	
[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.	Meets criteria>>	398	603	6.08E+02	217
[b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).	total screened with AIM	561	6.00E+00	moderate	42.00
Footnotes		>1000 ug/L	155.00	high-moderate	22.00
		>1 -1000 ug/L	282.00	low-moderate	53.00
		>0.001-<1 ug/L	107.00	low	61.00

CASRN	CASRN (without hyphens)	category	EcoSAR class
146832-03-3	146832033		
182635-99-0	182635990		Aliphatic amine

[a] Atmospheric oxidation half-lfe could not be estimated with AOPWIN.

[b] These are the production values for the five reporting years for the TSCA IUR (0.5 = 10-500 K; 1 = 500 K-1 M; 10 = 1-10 M; 50 = 10-50 M; 100 = 50-100 M; 500 = 100-500 M; 1000 = 500-1000 M lbs for the reporting year).

Footnotes			
	airbreather	71	
	neutral organics		330
	esters		46

Priorities	CASRN	CASRN (without hyphens)	Molstructure

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CASRN	Smiles	Class		VP est. (mmHg)	VP est. (Pa)
		P	19	3.11%	
		other	1	0.16%	
		3	610	100.00%	
	halogenated			61.80%	

CASRN	Atmospheric Oxidation $t_{1/2}$	LogK_{aw}	LogK_{ow}	LogK_{oa}	BCF	logBCF

CASRN	Comment	Neutral and non-polymer	Currently analysed in environme	Analysable using existing	Analysable by GC-MS after
	WELL MONITORED				
	SI analysable?			33	
				0.662295082	
	F degradation products				
	% of total F compounds				
	neutrals	473			
	phenols	58			
	acids	58			
	amines	16			

CASRN	Analysable by LC-MS/MS ESI	Probable degradation product	Analysable degradation product	Legacy and well	Pdt'n range (M lbs) 86[b]	Pdt'n range (M lbs) 90	Pdt'n range (M lbs) 94	Pdt'n range (M lbs) 98	Pdt'n range (M lbs) 02
				47	0.07704918				
	0.070491803								
	0.039344262								
				132					
				0.729281768					

CASRN	Pdt'n range (M lbs) 06	TSCA New Chemicals Program (meets	ECOSAR (lowest LC_{50} value for all species)	ECOSAR (species, duration, endpoint, predicted mg/L)	OncoLogic Concern Level
		<0.001 ug/L	59.00	marginal	38.00
			6.03E+02	high	1.00
					217.00
		>1000 ug/L	26%	moderate	0.19
		>1 -1000 ug/L	47%	high-moderate	0.10
		>0.001-<1 ug/L	18%	low-moderate	0.24
		<0.001 ug/L	10%	low	0.28
				marginal	0.18
				high	0.005

CASRN	CASRN (without hyphens)	category	EcoSAR class
	amines		21
	acid chloride/halide		16
	Peroxy Acids		5
	phenols		41
	others		149
			608