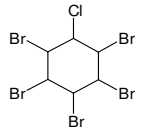
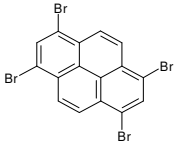
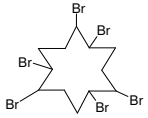
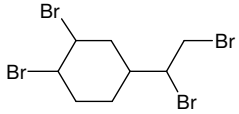
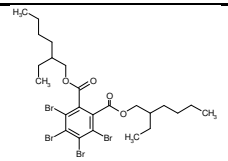
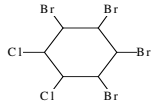
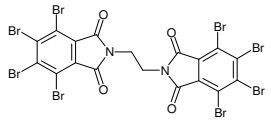
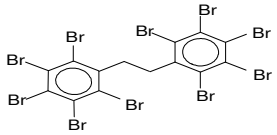
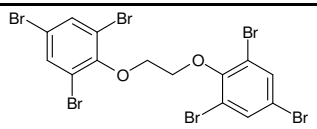
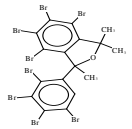
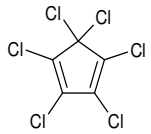
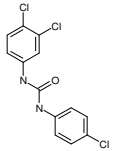
Top 50 Priorities

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
87843		Br	4.61E-04	15.71	-4.41	4.71	9.12	860	N	N	Y
128632		Br	5.41E-08	6.57	-5.07	8.49	13.56	2424	Y	N	Y
3194556		Br	2.24E-06	2.13	-4.15	7.74	11.89	6211	N	Y	Y
3322938		Br	1.40E-02	2.20	-2.77	5.24	8.01	2153	N	Y	Y
26040517		Br	2.28E-09	0.49	-4.91	11.95	16.86	3	N	N	Y
30554724		Br	1.12E-03	16.36	-3.92	4.62	8.54	716	N	N	Y

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
87843							0.5		0.5	–
128632					0.5	1	10		1	0.5
3194556					10	10	50	50	50	50
3322938					0.5	0.5	0.5	0.5	0.5	–
26040517			tetrabromo phthalic acid	Y	10	10	10	10	10	10
30554724					0.5	0.5	0.5	0.5		–

CAS # without hyphens	Smiles	Comment
87843	BrC(C(C(Br)C(Br)C1Br)Cl)C1Br	Analysable with HCHs
128632	c(c(c(c(cc1Br)Br)cc2)c1cc3)(c2c(cc4Br)Br)c34	Tetrabromopyrene. Possible intermediate rather than BFR. Could be very light sensitive
3194556	BrC(C(Br)CCC(Br)C(Br)CCC(Br)C(Br)C1)C1	Hexabromocyclododecane. Limited Great Lakes measurements. Possible penta BDE replacement
3322938	BrCC(Br)C(CCC(Br)C1Br)C1	Limited environmental measurements. Currently being detected e.g. herring gull eggs. 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 Q
26040517	O=C(OCC(CCCC)CC)c(c(c(c(c1Br)Br)Br)C(=O)OCC(CCCC)CC)c1Br	Possible PentaBDE replacement; hydrolysis to diacid - LOGKOW 4.6 - looks very persistent. ; may be amendable to GC-MS
30554724	BrC1C(C(C(C(C1Br)Br)Cl)Cl)Br	Analysable with other bromo/chlorobenzenes

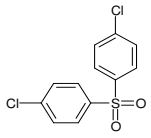
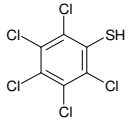
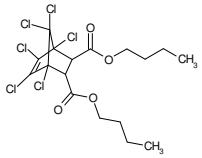
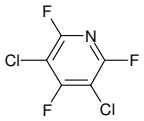
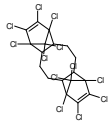
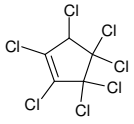
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
87843	LD polystyrene foam: 1 – 2 parts of [3194-55-6], pentabromomonochlorocyclohexane (Dow Chemical 651P) [87-84-3], & [3322-93-8] produce foam meets building code in US - Ullmann Encylo., Zitko DETECTION OF BROMINATED FLAME RETARDANTS IN	Accustandard
128632	No K-O, Ullmanns, EFDB, TOXNET Organic electroluminescent (EL) displays - may intermediate, next-generation display capable of replacing LCDs (liquid crystal displays) European Patent	Wellington Labs
3194556	use as an additive flame retardant for extruded and expanded polystyrene foam, crystal and high-impact polystyrene, SAN (Styrene-AcryloNitrile) resins, adhesives, and coatings. 3rd most widely used BFR, Several EST	Wellington Labs
3322938	Additive flame retardant in polystyrene, polyurethane, and polyvinyl chloride - Ashford 1994 Tomy et al 2008 detection in Beluga whales bubber	Wellington Labs
26040517	LOGKOW 11.95 but probably hydrolysis to diacid - LOGKOW 4.6 - looks very persistent. Mack (2004) FRP-45 (Unitex) DP45 (Great Lakes) - flame-retardant plasticizer (45% bromine) - main application in PVC coatings	Wellington Labs
30554724	No KO, Ullmann, EFDB, HSDB. May not have been in commerce for some time. Is on DSL but was not categorized in.	No source identified

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
32588764		Br	3.39E-20	0.27	-18.83	9.80	28.63	10	N	N	Y
84852539		Br	2.53E-11	4.50	-5.92	13.64	19.56	3	N	Y	Y
37853591		Br	3.17E-08	0.72	-6.52	9.15	15.67	74	N	Y	Y
155613937		Br	1.64E-10	6.20	-6.91	11.80	18.71	1	N	N	Y
77474		Cl	6.51E+00	26.99	-1.06	4.63	5.69	1516	Y	N	Y
101202		Cl	4.81E-07	0.50	-8.73	4.90	13.63	1187	N	N	Y

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
32588764			tetrabromophthalic acid	Y	10	1	10	50	10	10
84852539										–
37853591			Tribromophenol	Y	50	50	50	10	10	10
155613937								10	0.5	–
77474					50	50	50	50	50	50
101202					0.5	10	10	1	10	0.5

CAS # without hyphens	Smiles	Comment
32588764	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	should be analysable under similar conditions to BTBPE
84852539	Brc2c(Br)c(Br)c(CCc1c(Br)c(Br)c(Br)c(Br)c1Br)c(Br)c2Br	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
37853591	O(c(c(cc(c1)Br)Br)c1Br)CCOc(c(cc(c2)Br)Br)c2Br	Replacement for Penta and Decabromo BDEs. Limited measurements in the Great lakes region. Another BFR Prod 1-10M last two years. Currently being detected e.g. herring gull eggs
155613937	CC3(C)OC(C)(c1cc(Br)c(Br)c(Br)c1Br)c2c(Br)c(Br)c(Br)c(Br)c23	Octabromo-1,1,3-trimethyl-3-phenyl indan; should be analysable by GC MS with PBDEs
77474	C(=C(C(=C1Cl)Cl)Cl)(C1(Cl)Cl)Cl	Hexachlorocyclopentadiene. 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??
101202	O=C(Nc(ccc(c1)Cl)c1)Nc(ccc(c2Cl)Cl)c2	Triclocarban. Microbicide. Looks very persistent. Some environmental measurements in the Great Lakes

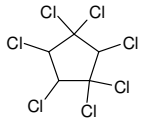
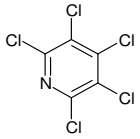
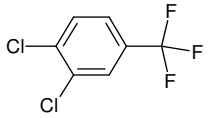
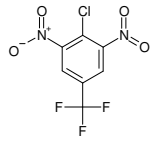
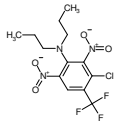
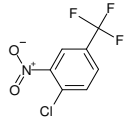
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
32588764	added June 08 because of ongoing Canadian risk assessment and evidence of HPV. Saytex BT-93 flame retardant, in many systems more effective than decabromodiphenyl oxide even though lower bromine content.	SAYTEX® BT-93W
84852539	added June 08 because of detection in HG eggs. KO – Mack (2004) The additive ethane-1,2-bis(pentabromophenyl) (SAYTEX 8010) [84852-53-9] is prepared by the bromination of diphenyl ethane in neat bromine (bromine is	Wellington Labs
37853591	Another BFR Prod 1-10M last two years. Tree bark Zhu & Hites, EST40:3711-16(2006); Atmos above Great Lakes Venier & Hites EST 42: 4745-4751 (2008) KO - Additive BFR, Good UV stability - used in ABS resins	Wellington Labs
155613937	EFDB, HSDB, KO - Additive BFR. Produced by dimerization of alpha-methylstyrene and then bromination. Can't form brominated dioxins and furans.	Wellington Labs
77474	Analog search maleic anhydride analog (chlorendic anhydride) - 1M - 10M, acid varies 2002 500K-1M, 2-EH ester of acid 10K-500K, Dichlorane Plus 1M-10M, Heptachlorocyclopentene - 1M - 10M but no	Aldrich H6002
101202	GLEDHILL WE; BIODEGRADATION OF 3,4,4'-TRICHLOROCARBANILIDE, TCC, IN SEWAGE & ACTIVATED SLUDGE; WATER RES 9(7) 649 (1975) 50% 14CO2 evol 2-4 weeks, may not be P; KO - Triclocarban -	Aldrich 105937

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
80079		Cl	0.0001079	218.8586	-5.2519	3.9	5.75756	199.5	Y	N	Y
133493		Cl	2.49E-02	76.72	-2.32	5.91	8.23	7066	Y?	N	Y
1770805		Cl	1.627E-05	320.20	6.28	7.25	0.97	29340	Y	N	Y
1737935		Cl	2.08E+02	172.54	-4.60	2.69	7.29	24	Y	N	Y
13560899		Cl	9.41E-08	160.10	-3.52	11.27	14.79	1	N	Y	Y
62111471		Cl	6.76E-01	2.66	-1.99	4.44	6.43	521	Y	N	Y

CAS # without hyphens	Analysable by GC-MS after derivatization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
80079					10	10	50	50	50	50
133493					1	1	1	0.5	0.5	–
1770805			hexachlorocyclopentadiene-phthalate					0.5	0.5	–
1737935							0.5	10	10	10
13560899					10	10	10	10	10	10
62111471							10	10	10	–

CAS # without hyphens	Smiles	Comment
80079	O=S(=O)(c(ccc(c1)Cl)c1)c(ccc(c2)Cl)c2	bis-2chlorophenyl sulfone has been reported in wildlife by Olsson and Bergman 1995; ppm levels in guillemot eggs in the Baltic
133493	Sc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl	May be analysed by GC-MS. Not HPV
1770805	CCCCOC(=O)C1C(C(=O)OCCCC)C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl	Dibutyl chlorendate, flame retardant. May be amenable to GC-MS if esters are stable.
1737935	Clc(c(F)nc1F)c(F)c1Cl	very persistent (five halogens on a pyridine ring - KOWWIN only 2.69 - use as chemical intermediate; may be occupational exposure measurements
13560899	C(=C(C(C1(Cl)Cl)(C(C2CCC(C(C(=C(C34Cl)Cl)C	Dechlordane Plus ®. Has been measured in Great Lakes samples.
62111471	ClC1(C(C(Cl)C(=C1Cl)Cl)(Cl)Cl)Cl	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. Use - olefin - polymer monomer? USEPA HPV challenge program - no sponsored

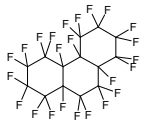
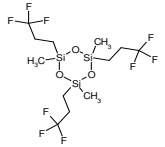
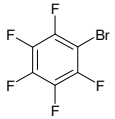
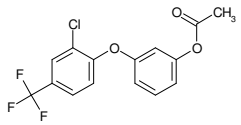
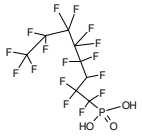
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
80079	Added to priority list due to widespread detection in the Baltic and in the north Atlantic (Jörundsdóttir et al. 2006; Norstrom et al. 2004) and identified in Great Lakes herring gull eggs (Letcher et al Anal Chem 1995)	Aldrich 51378
133493	Probably P&B; KO: Peptizing agent (reduce viscosity) for natural and synthetic rubber	Supelco MET690B
1770805	added June 08 because of high predicted BCF. Maybe P - esters will probably chemically hydrolyze. Diacid less B	Dow Corning MOLYKOTE(R) G 68
1737935	very persistent (five halogens on a pyridine ring - KOWWIN only 2.69; 3,5-Dichloro-2,4,6-trifluoropyridine is used to prepare the herbicides haloxydine [2693-61-0] and fluroxypyr-(1-methylheptyl) [81406-37-3]	Sigma-Aldrich 248010
13560899	Dechlorane-Plus; use as a flame retardant; detected in water, sediment, air, and fish samples - Hoh E et al 2006; Venier and Hites (2008) detected air above Great Lakes	Wellington Labs
62111471	Not in KO or Ullmann, polymer monomer? Intermdiate for hexachlorocyclopentadiene	No source identified

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
68258902		Cl	3.39E-01	93.49	-2.56	4.03	6.59	253	Y	N	Y
68412408		Cl	1.05E-01	974.13	-0.59	4.03	4.62	104	Y	N	Y
328847		F	1.76E+02	132.87	0.02	4.24	4.22	370	Y	N	Y
393759		F	5.08E-02	16206.04	-4.66	3.24	7.90	17	Y	N	Y
29091201		F	4.69E-05	5.35	-2.19	5.96	4.76	7688	Y?	N	Y
121175		F	15.73	3724.92	-2.25	3.42	2.28	86	Y	N	Y

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
68258902							50	500	50	–
68412408					10	10	10	10	10	10
328847					10	10	10	10	10	0.5
393759					1	10	10			0.5
29091201					0.5		1	1		–
121175					0.5	0.5			0.5	–

CAS # without hyphens	Smiles	Comment
68258902	ClC1(C(C(C(C1Cl)Cl)(Cl)Cl)Cl)Cl	One of a series of chlorinated cyclopentane derivatives; likely easily analysed by GC analysis. Use?
68412408	n1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	Like other chloropyridines, looks persistent. Probably persistent. Uses - pesticide intermediate?
328847	FC(F)(F)c(ccc(c1Cl)Cl)c1	3,4-Dichlorobenzotrifluoride. Looks very P, pesticide/drug intermediate? See also 78068-85-6
393759	N(=O)(=O)c1c(Cl)c(N(=O)(=O))cc(C(F)(F)F)c1	1-Chloro-2,6-Dinitro-4-(Trifluoromethyl) Benzene. Predicted to be very P, no recent Production
29091201	N(=O)(=O)c1c(c(c(c(c1)C(F)(F)F)Cl)N(=O)(=O))N(CCC)CCC	
121175	O=N(=O)c(c(ccc1C(F)(F)F)Cl)c1	Analog of 393759

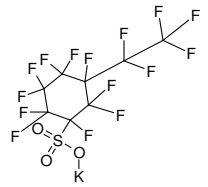
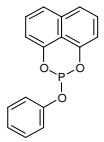
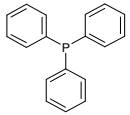
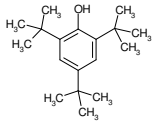
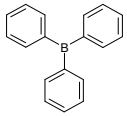
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
68258902	No use in KO or Ullmann. KO - Cheug (2001) Tetrachlorocyclopentane is produced first, by chlorine addition, and is then converted to octachlorocyclopentane[no hepta?] by catalytic chlorination over arsenious oxide or	No source identified
68412408	No use in KO or Ullmann for CAS #; Probably persistent. Uses - KO Scriven and Murugan (2005) 2,3,5,6-Tetrachloropyridine [2402-79-1] used in the synthesis of the insecticide chlorpyrifos [2921-88-2] (43)(57), and the	Aldrich 138002
328847	KO Boudakian, M.M. (2000) – physical properties of commercial chemicals listed Ullmann - Siegemund et al. (2000) 4-Chlorobenzotrifluoride and 3,4-dichlo-robenzotrifluoride are intermediates for	Aldrich 235806
393759	KO Boudakian, M.M. (2000) – physical properties of commercial chemicals listed Ullmann - Siegemund et al. (2000) The key intermediate, 4-chloro-3,5-dinitrobenzotrifluoride [393-75-9], is obtained by	Aldrich 197017
29091201	added June 08 because of relatively high predicted BCF. 'KO - nothing Ullmann - nothing	No source identified
121175	added June 08 because of high predicted persistence. 'KO – Boudakian (2000) Nitration provides either 4-chloro-3-nitrobenzotrifluoride [121-17-5] (one-step) or 4-chloro-3,5-dinitrobenzotrifluoride [393-75-9] (two-step) for	Aldrich C60600

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
306912		F	42.80	very long	8.78	9.58	-2.60	19	N	N	Y
2374143		F	40.40	2.39	3.84	8.66	4.82	343	N	N	Y
344047		F	971.92	1025.74	-0.72	3.88	1.21	196	Y	N	Y
50594779		F	1.88E-03	2.56	-3.43	4.41	7.84	500	N?	N	Y
68412680		F	6.95E-02	38.20	-3.36	6.48	9.84	19510	N	N	N

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
306912					0.5	0.5		0.5		–
2374143					10	1	1	10	10	0.5
344047								0.5		–
50594779			halogenated diphenyl(ol)	Y	1	10		10	10	–
68412680		Y	PFOA/PFNA	Y				0.5	0.5	–

CAS # without hyphens	Smiles	Comment
306912	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)))	Represents a class of perfluorinated cyclics which are likely very persistent. Low predicted B. Relatively volatile. See also 306-94-5 (perfluoromethyldecalin i.e. perfluorinated methylnaphthalene derivative
2374143	FC(CC[Si]1(O[Si](O[Si](O1)(CCC(F)(F)F)C)(CCC(F)(F)F)C)C)(F)F	Fluorinated cyclic siloxane. May be analysable with other cyclic siloxanes by GC-MS
344047	Fc(c(c(F)c(F)c1F)Br)c1F	
50594779	O=C(Oc(cc(Oc(c(cc(c1)C(F)(F)F)Cl)c1)cc2)c2)C	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
68412680	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	Perfluoroalkyl (C6-C12) phosphonic acid . May be analysable as is by LC-MS. May degrade to PFNA or PFOA

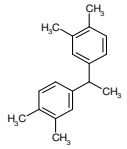
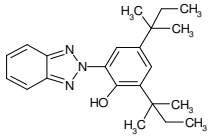
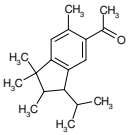
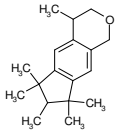
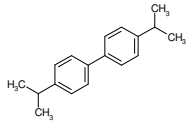
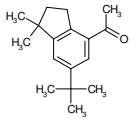
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
306912	added June 08 because of very high persistence. 'Ullmann – Siegemund et al. (2000) 624 PP11 Flutec PP11 finds many applications in the electronics industry, including as a fluid for vapour phase soldering,	www.fluorochem
2374143	industrial monomer is 2,4,6-trimethyl-2,4,6-tris-(3,3,3-trifluoropropyl)cyclotrisiloxane [2374-14-3], which is produced by the hydrosilylation of 3,3,3-trifluoropropene [677-21-4] with methyldichlorosilane [75-54-7], c	http://www.alfa.com; Item# L16680
344047	added June 08 because of high predicted persistence. 'KO – Boudakian (2000) Decafluorobiphenyl [434-90-2 – not in DSL/IUR chemicals], C6F5C6F5 (mol wt, 334.1; mp, 68°C; bp, 206°C), can be prepared by Ullmann	Aldrich B75158
50594779	KO – nothing Ullmann – nothing	http://www.honestjoy.cn/cas/O16.htm
68412680	KO – nothing Ullmann – nothing	Mason Chemical Co

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
67584423		F	2.09E-07	very long	-9.83	0.47	10.30	3	N	N	N
101020		Non-halo	1.02E-02	0.99	-4.66	6.62	11.28	25170	Y	N	Y
603350		Non-halo	1.36E-03	1.83	-6.03	5.02	11.05	4801	Y	N	Y
732263		Non-halo	2.67E-02	0.67	-3.40	6.39	9.79	3282	Y	N	N
960714		Non-halo	3.29E-03	1.83	-3.00	5.52	8.52	3558	Y	N	?

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
67584423		Y					0.5	0.5		–
101020			Triphenyl phosphate?	Y	50	50	50	50	50	50
603350					1	10	10	10	10	1
732263	Y				10	10	10	10	50	50
960714					10	10	10	50	10	10

CAS # without hyphens	Smiles	Comment
67584423	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)F)O[K]	Perfluoro-4-ethylcyclohexane sulfonate. May be analysable along with other perfluoroalkane sulfonates. See precursor 68156-06-9 and analog 68318-34-3
101020	O(c(cccc1)c1)P(Oc(cccc2)c2)Oc(cccc3)c3	Triphenyl phosphite - 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
603350	c(P(c(cccc1)c1)c(cccc2)c2)(cccc3)c3	Triphenylphosphine
732263	Oc(c(cc(c1)C(C)(C)C)C(C)(C)C)c1C(C)(C)C	2,4,6-Tri-tert-butylphenol ; experimental P, like BHT oxidize to quinone?
960714	c1ccc(cc1)B(c2ccccc2)c3ccccc3	Check stability of aromatic boranes

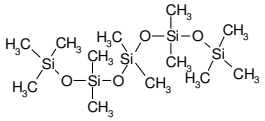
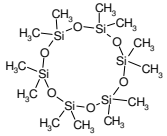
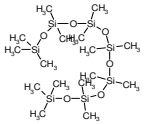
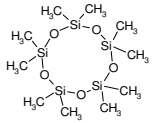
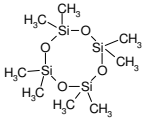
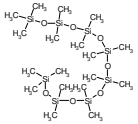
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
67584423	added June 08 because of similarly to PFOS and lack of measurements. 'KO – nothing Ullmann – nothingProduced by Miteni in Italy. All new users must have a Significant Us Report in the US. According to a chemist at MIC the only known use is in hydraulic	MIC Specialty Chemicals
101020	HAZARD INFORMATION PROFILE OF TRIPHENYL PHOSPHITE – major use – chemical intermediate in manufacture of phosphate stabilizers/antioxidants. Hydrolyzes in water – times of 80 min, 24 hrs, and 5 days	Aldrich T84654
603350	Ullmann - Svara et al. (2006) Triphenylphosphine, which is important as a catalyst ligand and as an intermediate in the synthesis of Wittig reagents, is also produced by BASF in a reaction analogous to the Wurtz	Sigma-Aldrich T84409
732263	KO – nothing Ullmann – Fiege et al (2000) 2,4,6-Tri-tert-butylphenol is the starting material for the synthesis of 2,6-di-tert-butyl-4-methoxyphenol [489-01-0] which is a powerful antioxidant.	Aldrich T49409
960714	KO – nothing Ullmann – Brotherton et al. (2000) Triarylboranes are generally solid, less sensitive to oxygen, and also unreactive with water. The amine complexes of triarylboranes	Fluka 92985

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
1742149		Non-halo	9.67E-03	0.33	-1.41	6.34	7.75	15170	N	N	Y
25973551		Non-halo	2.57E-08	0.68	-10.57	7.25	17.82	10350	N	N	N
68140487		Non-halo	9.11E-03	0.55	-2.76	6.31	9.07	2080	N	Y	Y
1222055		Non-halo	1.17E-02	0.28	-2.27	6.26	8.53	13200	N	Y	Y
69009901		Non-halo	9.80E-03	0.84	-1.20	6.67	7.87	27240	N	N	Y
13171001		Non-halo	1.92E-02	1.44	-2.75	5.93	8.68	1057	N	N	Y

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
1742149							10	10	10	–
25973551	Y				10	10	10	10	10	10
68140487					0.5	0.5	0.5	0.5	0.5	0.5
1222055					1	10	10	10	10	10
69009901							10	10	10	10
13171001					0.5	0.5	0.5	0.5	0.5	-

CAS # without hyphens	Smiles	Comment
1742149	c(ccc(c1C)C)(c1)C(c(ccc(c2C)C)c2)C	highly substituted, P?
25973551	Oc(c(cc(c1)C(CC)(C)C)C(CC)(C)C)c1n(nc(c2ccc3)c3)n2	UV absorber used in rubber, polymer industry. Likely analysable by GC-MS after derivatization or possibly by LC-MS (ESI)
68140487	O=C(c(c(cc(c1C(C2C)C(C)C)C2(C)C)C)c1)C	musk methyl ketone. Great Lakes measurements. Analysable with other hydrocarbons/substituted benzenes by GC-MS
1222055	O(CC(c(c1cc(c2C(C3C)(C)C)C3(C)C)c2)C)C1	Galoxolide. Highly branched cyclopentyl ring fused on benzene - musk? Use? LOGKOW 6.26 - could be P. Limited monitoring - mainly for sediments and near shore waters/effluents
69009901	CC(c1ccc(cc1)c2ccc(cc2)C(C)C)C	Substituted biphenyl. Not P but could be B. Analysable with other aromatic hydrocarbons.
13171001	O=C(c(c(c(cc1C(C)(C)C)C(C2)(C)C)C2)c1)C	musk dimethyl indane. Concentrations increasing in L Ontario sediment (Peck et al EST 2006). Predicted high toxicity using ECOSAR

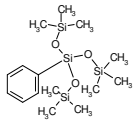
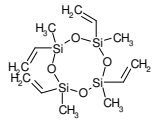
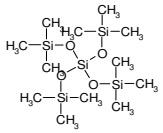
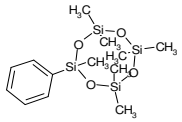
CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
1742149	KO – nothing; Ullmann – nothing	http://www.yickvic.com/products-cc000b.html
25973551	tert-amylphenol is in the production of UV stabilizers; the principal one is a benzotriazole-based uv absorber, 2-(2'-hydroxy-3',5'-di-tert-amylphenyl)-5-chlorobenzotriazole [25973-55-1], which is widely us	Aldrich 422746
68140487	added June 08 because of detection in abiotic media (Peck et al EST 2006) and high predicted ecotox	Promochem
1222055	added June 08 because of high predicted BCF and detection in abiotic media at relatively high conc (Peck et al EST 2006). Musk - 20% detected; Kolpin et al. 2004; HHCB	Aldrich W520608
69009901	KO- nothing Ullmann – nothing	No source identified
13171001	added June 08 because of detection in abiotic media (Peck et al EST 2006) and high predicted ecotox. (ADBI - Celestolide) - musk fragrance that does not occur in nature Fahlbusch et al. (2002)	Promochem

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
141639		Si	9.39E+00	5.96	1.51	6.52	5.01	8318	N	N	Y
540976		Si	4.73E+00	5.96	0.83	6.33	5.50	14890	N	Y	Y
541015		Si	1.23E+00	4.47	0.78	7.69	6.91	34360	N	Y	Y
541026		Si	2.91E+01	7.15	0.69	5.71	5.02	2014	N	Y	Y
556672		Si	1.57E+02	8.94	0.55	5.09	4.54	1687	N	Y	Y
556694		Si	1.39E+00	3.97	0.92	8.28	7.36	7096	N	N	Y

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
141639					0.5	0.5	0.5	0.5	0.5	
540976					0.5	10	10	10	50	
541015									0.5	
541026					50	50	50	100	500	
556672					500	500	500	500	500	
556694									0.5	

CAS # without hyphens	Smiles	Comment
141639	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	Dodecamethylpentasiloxane. May have similar properties to D5 cyclic siloxane which has been analysed by GC-MS
540976	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	D6. Methodology under development; some environmental measurements in the Great Lakes
541015	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	Methodology under development; some environmental measurements
541026	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	D5. Methodology under development; some environmental measurements in the Great Lakes
556672	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	D4. Methodology under development; some environmental measurements in the Great Lakes
556694	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	Methodology under development; some environmental measurements

CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
141639	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
540976	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
541015	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
541026	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
556672	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
556694	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined

CAS # without hyphens	Molstructure	Class	VP est (Pa)	Atmos Oxid'n t1/2 (days)	Log Kaw	log Kow	Log Koa	BCF	Chemical intermediate?	Currently analysed in environmental monitoring or research programs in the Great Lakes	Analysable using existing methods for neutral POPs or other neutrals such as pesticides, i.e. no derivatization
2116849		Si	3.13E-01	3.24	0.16	7.15	6.99	40260	N	N	Y
2554065		Si	1.43E+01	0.10	0.56	6.51	5.95	20410	N	N	Y?
3555473		Si	2.01E+01	5.96	1.51	6.52	5.01	20860	N	N	Y
10448096		Si	3.41E-01	3.57	-0.66	6.30	6.96	14260	N	N	Y

CAS # without hyphens	Analysable by GC-MS after deriva-tization	Analysable by LC-MS/MS ESI mode (anionic) or positive (cation) mode	Probable degradation product	Analysable degradation product	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	Pdt'n range (M lbs) 06
2116849					0.5	0.5	1	0.5		
2554065					0.5	0.5	0.5	0.5	0.5	
3555473										
10448096										

CAS # without hyphens	Smiles	Comment
2116849	C[Si](O[Si](c1ccccc1)(O[Si](C)(C)C)O[Si](C)(C)C)(C)C	May be analysable with similar methodology as cyclic siloxanes
2554065	C=C[Si]1(O[Si](O[Si](O[Si](O1)(C=C)C)(C=C)C)(C=C)C)C	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
3555473	[Si](O[Si](O[Si](C)(C)C)(O[Si](C)(C)C)O[Si](C)(C)C)(C)(C)C	Tetrakis(trimethylsilyloxy)silane or Trisiloxane. Used as a pesticide adjuvant. May be analysable by GC-MS although highly volatile similar to D6.
10448096	C[Si]1(C2=CC=CC=C2)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1	heptamethyl-phenyl-cyclotetrasiloxane. Should be analysable by GC-MS similar to cyclic siloxanes

CAS # without hyphens	Comments on revised list (July 2008 & March 2009) from Howard and Muir	Likely source of analytical standards
2116849	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
2554065	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
3555473	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined
10448096	Not recommended for fish monitoring until analytical methodology is better developed and background contamination issues are resolved	Not determined