An Act to Protect Children, Families and Firefighters from Harmful Flame Retardants
Proposed Additional CAS numbers/Isomers/Analogues
of the 11 Flame Retardants Identified in the Law

Mass Act to Protect Children, Families, and Firefighters from Harmful Flame Retardants (Mass. Gen. Laws ch 21A, section 28 (2020), Regulations at 310 CMR 78.00) and Background Document

Note: Definitions requested by the Science Advisory Board (SAB) and Questions from the Department of Environmental Protection (DEP) for the SAB are provided in a companion document, "Definitions and Questions."

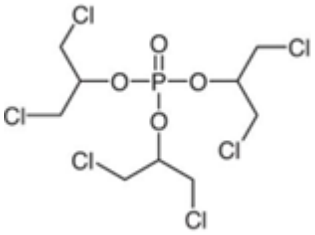
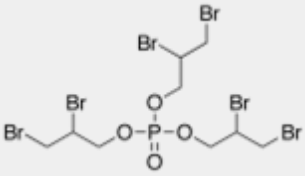
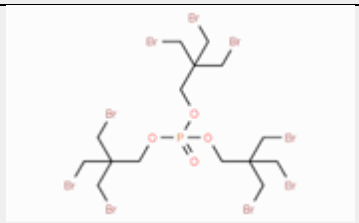
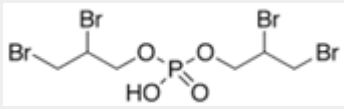
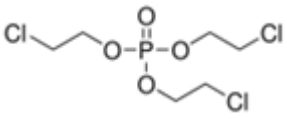
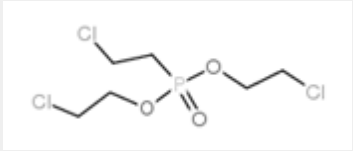
The Flame Retardant Chemicals

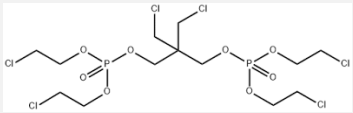
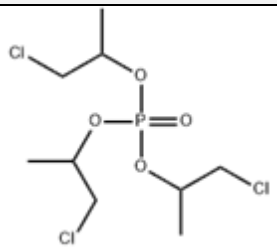
The 11 chemicals prohibited in the law "or (their) chemical analogue":

(i) Tris(1,3-dichloro-2-propyl)phosphate (TDCPP) (CAS 13674–87–8)
(ii) Tris(2-chloroethyl)phosphate (TCEP) (CAS 115–96–8)
(iii) Antimony trioxide (CAS 1309–64–4)
(iv) Hexabromocyclododecane (HBCD) (CAS 25637–99–4)
(v) Bis(2-Ethylhexyl)-3,4,5,6- tetrabromophthalate (TBPH) (CAS 26040–51–7)
(vi) 2-Ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB) (CAS 183658– 27–7)
(vii) Chlorinated paraffins (CAS 85535–84–8)
(viii) Tris (1-chloro-2-propyl) phosphate (TCPP) (CAS 13674–84–5)
(ix) PentaBDE (CAS 32534-81-9)
(x) OctaBDE (CAS 32536-52-0)
(xi) Tetrabromobisphenol A (TBBPA) (CAS 79-94-7)

In 2019 the National Academies of Sciences (NAS) published their report on work to develop a class approach to assessing organohalogen flame retardants. The 11 chemicals in the law are members of 6 NAS subclasses (plus one additional "inorganic" subclass). Additional CAS numbers, positional isomers, diastereomers and analogues proposed are shown below for each of these 7 subclasses.

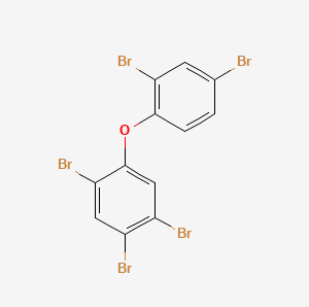
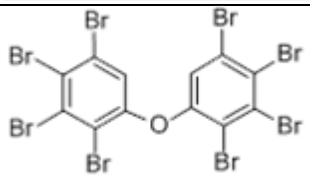
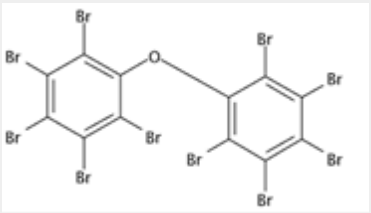
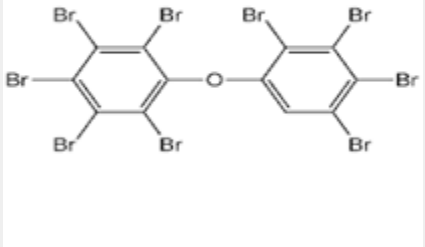
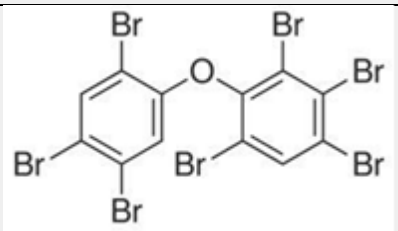
NAS Subclass 1: Polyhalogenated Organophosphates

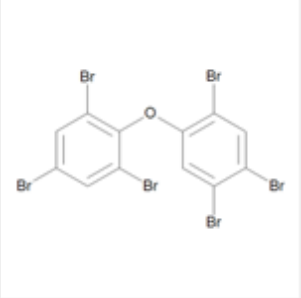
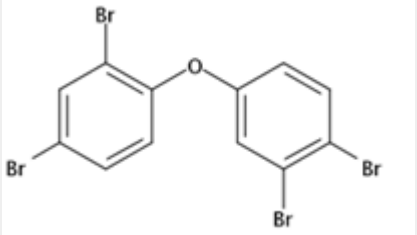
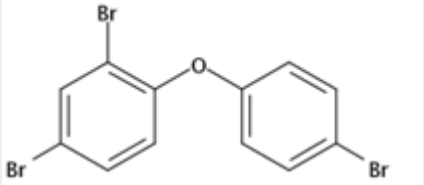
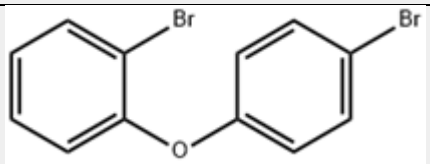
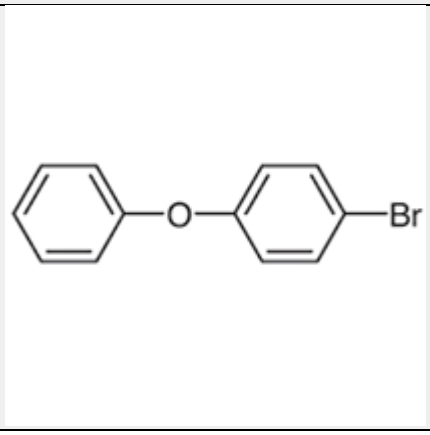
Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261 and potential Analogues	Chemical Structure	Difference from chemical identified in the law
(i) Tris(1,3-dichloro-2-propyl)phosphate* (TDCPP) 13674–87–8 $C_9H_{15}Cl_6O_4P$		Included in MA 310 CMR 78.00
Potential Analogue 1: Tris(2,3-dibromopropyl)phosphate (TDBPP) "Brominated tris" or "Tris" 126-72-7 $C_9H_{15}Br_6O_4P$		substitution of bromines for chlorines
Potential Analogue 2: Tris(tribromoneopentyl) phosphate 19186-97-1 $C_{15}H_{24}Br_9O_4P$		addition of methyl group to each chain, substitution of bromines for chlorines, addition of 3 bromines
Potential Analogue 3: Bis(2,3-dibromopropyl)phosphate 5412-25-9 $C_6H_{11}Br_4O_4P$		substitution of bromines for chlorines and one propyl group hydrolyzed (hydrolysis product of Potential Analogue 1)
(ii) Tris(2-chloroethyl)phosphate (TCEP) 115–96–8 $C_6H_{12}Cl_3O_4P$		Included in MA 310 CMR 78.00
Potential Analogue 1: Bis(2-chloroethyl)2-chloroethyphosphonate 6294-34-4 $C_6H_{12}Cl_3O_3P$		ethyl group bonded directly to P phosphonate, not phosphate

Potential Analogue 2: "V6" 2,2-bis(chloromethyl)-propane-1,3-diyltetrakis(2-chloroethyl) bisphosphate 38051-10-4 $C_{13}H_{24}Cl_6O_8P_2$		Two TCEP together
(viii) **Tris (1-chloro-2-propyl) phosphate**** (TCPP) 13674–84–5 $C_9H_{18}Cl_3O_4P$		Included in MA 310 CMR 78.00

Note: Positional isomer CAS numbers listed below may not be exhaustive.
* Positional isomer of TDCPP: Tris(2,3-dichloropropyl)phosphate (78-43-3)
**Positional isomers of TCPP: Tris(2-chloropropyl)phosphate (6145-73-9), Tris(3-chloropropyl)phosphate (26248-87-3 and 1067-98-7), Bis(2-chloropropyl)(2-chloro-1-methylethyl phosphate) (76649-15-5), Bis(2-chloro–1-methylethyl)(2-chloropropyl)phosphate (76025-08-6), Bis(2-chloro-1-methylethyl)(3-chloro-1-propyl)phosphate (137909-40-1) not on PubChem, Bis(3-chloro-1-propyl)(2-chloro-1-methyl)phosphate (no CAS number)

NAS Subclass 2: Polyhalogenated Diphenyl Ethers

Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261 and potential Analogues	Chemical Structure	Difference from chemical identified in the law
(ix) Pentabromodiphenyl ether (PentaBDE)[1] 32534-81-9 $C_{12}H_5Br_5O$		Included in MA 310 CMR 78.00
(x) Octabromodiphenyl ether (OctaBDE)[2] 32536-52-0 $C_{12}H_2Br_8O$		Included in MA 310 CMR 78.00
Potential Analogue 1: Decabromodiphenyl ether (DecaBDE, BDE-209) 1163-19-5 $C_{12}Br_{10}O$		10 bromine
Potential Analogue 2: Nonabromodiphenyl ether[3] (BDE-206) 63387-28-0 $C_{12}HBr_9O$		9 bromine
Potential Analogue 3: Heptabromodiphenyl ether[4] (BDE-183) 207122-16-5 $C_{12}H_3Br_7O$		7 bromine

Potential Analogue 4: Hexabromodiphenyl ether[5] 446255-03-4 - BDE-148; $C_{12}H_4Br_6O$		6 bromine
Potential Analogue 5: Tetrabromodiphenyl ether[6] 5436-43-1 (BDE-47) $C_{12}H_6Br_4O$		4 bromine
Potential Analogue 6: Tribromodiphenyl ether[7] 147217-78-5; $C_{12}H_7Br_3O$		3 bromine
Potential Analogue 7: Dibromodiphenyl ether[8] 2050-47-7 (BDE-15) $C_{12}H_8Br_2O$		2 bromine
Potential Analogue 8: Monobromodiphenyl ether (4-bromodiphenyl ether)[9] 101-55-3 (BDE-3) $C_{12}H_9BrO$		1 bromine

Note: Positional isomer CAS numbers listed below are not exhaustive.

[1] CAS Number 32534-81-9 refers to 2,2'4,4',5-pentabromodiphenyl ether. 60348-60-9 (BDE-99) is also 2,2',4,4',5-pentabromodiphenyl ether. Positional isomer of PentaBDE: 189084-64-8 (BDE-100)

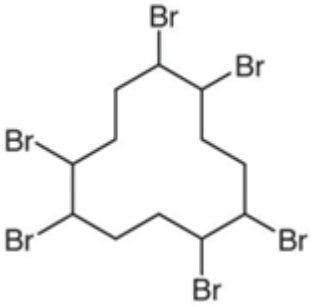
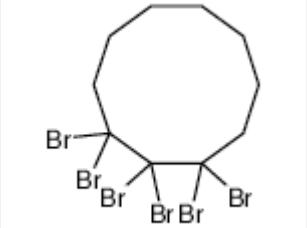
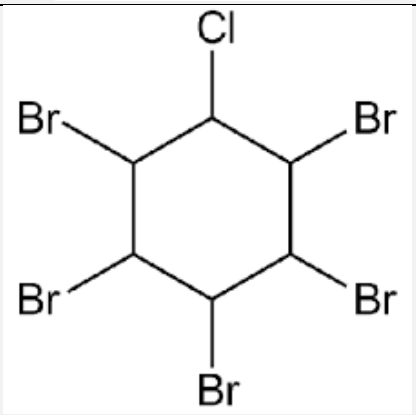
[2] CAS Number 32536-52-0 refers to 2,2'3,3',4,4',5,5'-octabromodipheyl ether. Positional isomers of OctaBDE: 117964-21-3, 85446-17-9, 67797-09-5, 446255-56-7, 446255-42-1, 446255-38-5, 337513-72-1

[3] Positional isomers of NonaBDE: 437701-78-5 (BDE-208); 437701-79-6 (BDE-207)

[4] Positional isomers of HeptaBDE: 189084-67-1 (BDE-181)

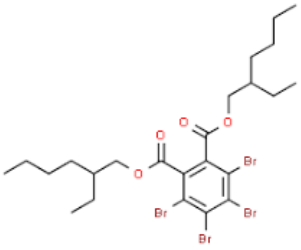
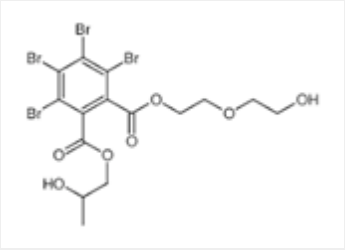
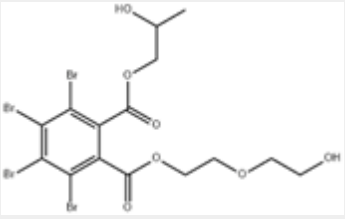
[5] Positional isomers of HexaBDE: 68631-49-2 (BDE-153); 207122-15-4 (BDE-154); 1620837-37-7; 36483-60-0
[6] Positional isomers of TetraBDE: 5436-43-1; 446254-27-9 (BDE-55);189084-61-5 (BDE-66); 40088-47-9; Not produced independently but a major component of Penta-BDE
[7] Positional isomers of TriBDE: 41318-75-6; 49690-94-0; 147217-75-2 (BDE-28); 189084-60-4 (BDE-32); 147217-73-0 (BDE-19), (also 113152-37-7; 1620837-31-1 deprecated)
[8] Positional isomers of DiBDE: 53563-56-7 (BDE-5); 446254-14-4 (BDE-5); 51452-87-0 (BDE-4); 6903-63-5 (BDE-11), 189084-59-1 (BDE-12); 171977-44-9 (BDE-7); 147217-72-9 (BDE-6); 147217-71-8 (BDE-8); 337513-66-3 (BDE-9); 51930-04-2 (BDE-10); 83694-71-7 (BDE-13)
[9] Positional isomers of MonoBDE: 7025-06-1 (BDE-1); 36563-47-0 (BDE-1)
(This subclass can be defined as: "brominated diphenyl ethers, including all positional isomers, where the number of bromines is one to ten.")

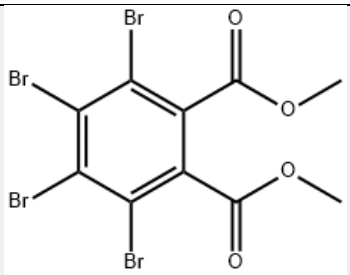
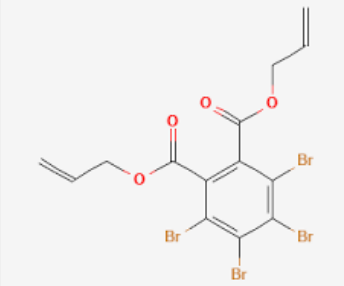
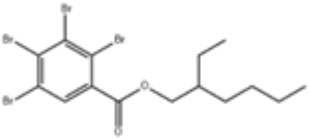
NAS Subclass 3: Polyhalogenated Alicycles

Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261 and potential Analogues	**Chemical Structure**	**Difference from chemical identified in the law**
(iv) **Hexabromocyclododecane** (HBCD)* 25637–99–4 $C_{12}H_{18}Br_6$		Included in MA 310 CMR 78.00
Potential Analogue 1: Hexabromocyclodecane** 25495-98-1 $C_{10}H_{14}Br_6$		2 fewer carbons on ring
Potential Analogue 2: 1,2,3,4,5-Pentabromo-6-chlorocyclohexane 87-84-3 $C_6H_6Br_5Cl$		Smaller ring, substitution of one halogen

Notes: *CAS number 25637-99-4 refers to 1,3,5,7,9,11-hexabromocyclododecane. HBCD has 16 stereoisomers. More common isomers are: 3194–55–6 and 1093632-34-8, a mixture of three main diastereomers. Also 134237-50-6, 678970-15-5, 138257-19-9 (alpha); 134237-51-7, 678970-16-6, 138257-18-8 (beta); 134237-52-8, 678970-17-7, 169102-57-2 (gamma). ** CAS 25495-98-1 refers to 1,1,2,2,3,3-hexabromocyclodecane. CAS 10364-34-8 is 1,2,3,4,7,8-Hexabromocyclodecane, a positional isomer. Isomer CAS numbers listed are not exhaustive.

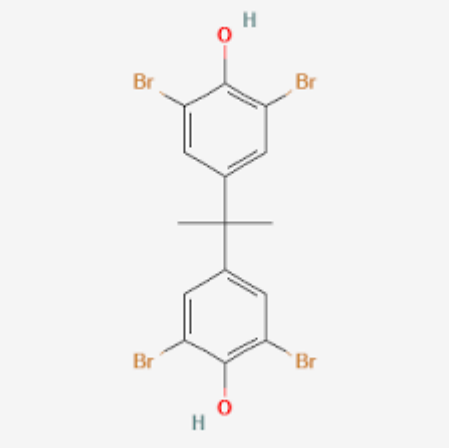
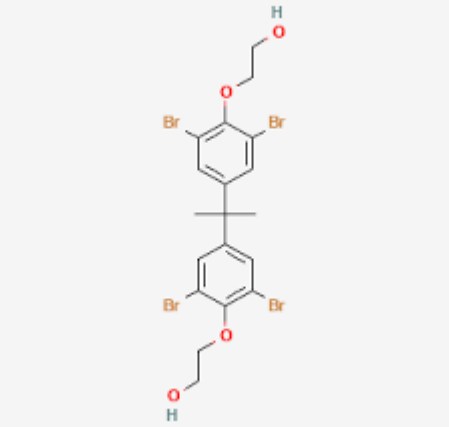
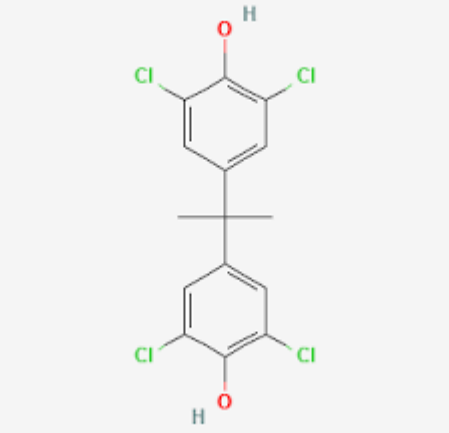
NAS Subclass 4: Polyhalogenated Phthalates/Benzoates/Imides

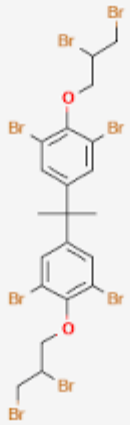
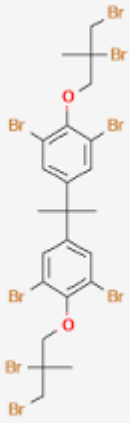
Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261 and potential Analogues	Chemical Structure	Difference from chemical identified in the law
(v) **Bis(2-Ethylhexyl)-3,4,5,6-tetrabromophthalate** (TBPH) 26040–51–7 $C_{24}H_{34}Br_4O_4$		Included in MA 310 CMR 78.00
Potential Analogue 1: 2-(2-hydroxyethoxy)ethyl-2-hyroxypropyl-3,4,5,6-tetrabromo phthalate 20566-35-2 $C_{15}H_{16}Br_4O_7$		Shorter, unbranched chains, additional O in chain, hydroxylated
Potential Analogue 2: 2-(2-hydroxyethoxy)ethyl-2-hyroxypropyl-3,4,5,6-tetrabromo phthalate mixed esters with diethylene and propylene glycol 77098-07-8 $C_{15}H_{20}Br_4O_9$		Similar to Potential Analogue 1 but mixture

Potential Analogue 3: Tetrabromophthalic acid dimethyl ester 55481-60-2 $C_{10}H_6Br_4O_4$		Absence of the alkyl chains
Potential Analogue 4: Diallyl tetrabromophthalate 49693-09-6 $C_{14}H_{10}Br_4O_4$		Diallyl groups on an ethyl chain
(vi) **2-Ethylhexyl-2,3,4,5-tetrabromobenzoate** (TBB) 183658– 27–7 $C_{15}H_{18}Br_4O_2$		Included in MA 310 CMR 78.00

Note: Positional isomer of TBPH - Dioctyl 3,4,5,6-tetrabromobenzene-1,2-dicarboxylate (CAS 56720-20-8); many other isomers of TBPH and TBB exist and some have patents for FR use but none have CAS numbers. Isomer CAS number listed may not be exhaustive.

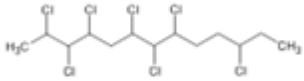
NAS Subclass 5: Polyhalogenated Bisphenol Aliphatics

Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261 and potential Analogues	Chemical Structure	Difference from chemical identified in the law
(xi) Tetrabromobisphenol A (TBBPA) 79-94-7 $C_{15}H_{12}Br_4O_2$		Included in MA 310 CMR 78.00
Potential Analogue 1: 4,4'-Isopropylidenebis[2-(2,6-dibromophenoxy)ethanol] 4162-45-2 $C_{19}H_{20}Br_4O_4$		addition of 2 ethyl groups; precursor of chemical identified in the law
Potential Analogue 2: Tetrachlorobisphenol A 79-95-8 $C_{15}H_{12}Cl_4O_2$		Substitution of Cl for Br

Potential Analogue 3: 2,2-Bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propane 21850-44-2 $C_{21}H_{20}Br_8O_2$		4 additional Br on propyl chain
Potential Analogue 4: 1,1'-(Isopropylidene)bis(3,5-dibromo-4-(2,3-dibromo-2-methylpropoxy)benzene) 97416-84-7 $C_{23}H_{24}Br_8O_2$		4 additional bromine on methylated chain

Notes: CAS 79-94-7 refers to 3,3’,5,5’ TBBPA. Isomers of TBBPA: 4,4’-TBBPA (CAS 121839-52-9) and 2,2'-Isopropylidenebis[4,6-dibromophenol] (CAS 97890-15-8). Isomer CAS numbers listed may not be exhaustive.

NAS Subclass 6: Polyhalogenated Aliphatic Chains

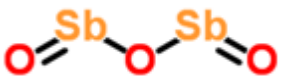
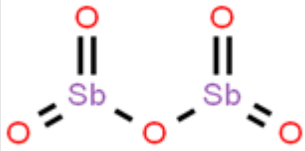
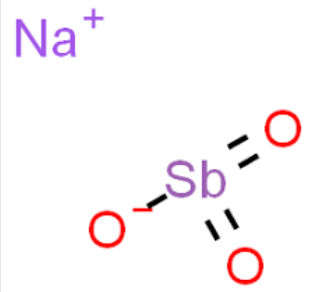
Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261	Chemical Structure	Status
(vii) **Chlorinated paraffins** 85535–84–8		Included in MA 310 CMR 78.00

Notes: Listed under TURA as "Polychlorinated alkanes, c10-c13" without CAS numbers. Many paraffin groups with different CAS numbers and definitions exist. Those listed below seem to fit or overlap with CAS 85535-84-8. This list is not exhaustive.

Chemical Name	CAS Number	Additional Information, Sources
Alkanes C_{10-13}, chloro ****CAS number listed in FR law**	**85535-84-8**	**Used by Stockholm Convention for Persistent Organic Pollutant (POP) designation; on European Chemicals Agency (ECHA) Substances of Very High Concern list 2008; DSL (Canadian Domestic Substances List); WA Chem of High Concern**
Alkanes, c10-12, chloro (60%)	108171-26-2	National Toxics Program (NTP) 1989 Report on Carcinogens, reasonably anticipated to be carcinogenic to humans; California Prop 65; MN Chem of High Concern; NJ RtK carcinogen; WA Chem of High Concern
Alkanes, C_{10-21}, chloro	84082-38-2	DSL; EU CAS registration; MN Chem of High Concern
Alkanes, C_{6-18}, chloro	68920-70-7	DSL PBiT; EU carcinogen; MN Chem of High Concern; ME; WA
Alkanes, chloro; chloroparaffins	61788-76-9	DSL; $C_{20\ o}$n PubChem; MN Chem of High Concern; OR High Priority Chem; WA Chem of High Concern to Children
Paraffin waxes, chloro	63449-39-8	DSL PBiT; C10-C16 on CAS Registry; C_{24}, FR use on PubChem; C_{22-30} 70% Cl on SDS; C_{18-28} on ECHA; MN Chem of High Concern; OSPAR; WA Chem of High Concern to Children
Alkanes, C_{14-17}, chloro 2,4,6,10,12,14-hexachloropentadecane	85535-85-9	EU CAS registration; C_{15} on PubChem; C_{14-17} on ECHA; MN Chem of High Concern

Sources: CPIA, Chlorinated Paraffins Industry Association, http://www.regnet.com/cpia/status_report.html, PubChem, ECHA, TSCA, CAS.org.

Subclass 7: Inorganic

Flame Retardants Regulated by MA Session Law - Acts of 2020 Chapter 261 and potential Analogues	Chemical Structure	Difference from chemical identified in the law
(iii) **Antimony trioxide** 1309–64–4 Sb_2O_3		Included in MA 310 CMR 78.00
Potential Analogue 1: Antimony pentoxide 1314-60-9 Sb_2O_5		Two additional oxygen; Sb in the +5 oxidation state
Potential Analogue 2: Sodium antimonate 33908-66-6 $Na.O_3Sb$		Sb in the +5 oxidation state

Notes: Listed under TURA as "antimony compounds." Additional CAS numbers for antimony trioxide follow. List may not be exhaustive. 12412-52-1: Diantimony trioxide (Senarmontite) ChemIDPlus, not on TSCA, 0 suppliers on CAS; 1317-98-2: Diantimony trioxide (Mineral Valentinite), not on TSCA, 0 suppliers on CAS; 1327-33-9: Diantimony trioxide (Senarmontite) ECHA.