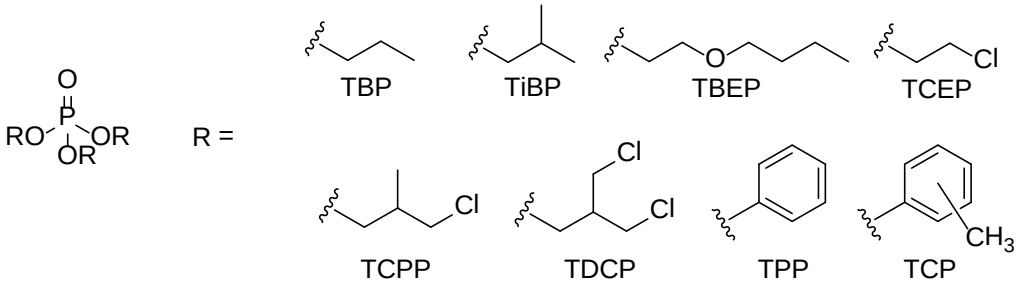
4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Phosphate esters are considered derivatives of the tri protic acid, phosphoric acid $O=P(OH)_3$, with the general formula of $R_xH_{3-x}PO_4$ where x=1 for mono, x=2 for di, and x=3 for triesters. Phosphorus has a high affinity for oxygen due to the difference in electronegativity (1.4), and consequently, the P=O bond possesses more σ character than π character. Therefore, the P=O bond, which dominates phosphate chemistry, can be more accurately depicted as a coordinate bond, $P\rightarrow O$, or as $P^+–O^-$. These phosphoric acid esters are often referred to as organophosphates. Trialkyl, triaryl, and trihaloalkyl/aryl, and mixed phosphate esters possess a central phosphorus atom with an oxidation state of +5 and an approximate tetrahedral geometry (Fee 2005; Gard 2005).



A wide array of substituents can occur as esters of phosphates. In many cases, all of the substituents are identical, as is the case for this profile; however, variable, mono-, di-, or tri-substituted as well as mixed substituents are common. The selected compounds, shown above, are trisubstituted, contain identical substituents, and fall into the following categories: alkyl (TnBP, TiBP), alkyl ether (TBEP), chloroalkyl (TCEP, TCPP, TDCP), and aryl (TPP, TCP) phosphate esters. Although the majority of selected compounds are discrete chemicals, commercial formulations of TCPP may contain minor amounts of structural isomers (NAS 2000). In addition, the commercial mixture of TCP as described here is an unspecified mixture of isomers, but commercial mixtures are predominantly meta and para isomers with less than 1% ortho (Winder and Balouet 2002). Table 4-1 lists common synonyms, trade names, and other pertinent information to identify the selected phosphate esters for this profile.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Table 4-2 lists important chemical and physical properties of the selected phosphate esters.

Table 4-1. Chemical Identity of Selected Phosphate Ester Flame Retardants[a]

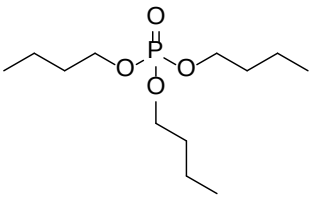
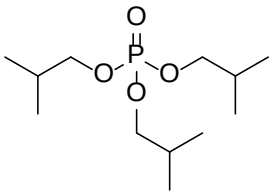
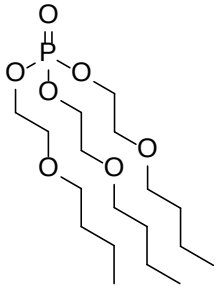
Characteristic	Tributyl phosphate	Triisobutyl phosphate	Tris(2-butoxyethyl) phosphate
Synonym(s)	TnBP; butyl phosphate; phosphoric acid tributyl ester; tri-n-butyl phosphate; tributoxyphosphine oxide	TiBP; isobutyl phosphate; phosphoric acid, tris(2-methylpropyl) ester	TBEP; tri(2-butoxyethyl) phosphate; tributoxyethyl phosphate; 2-butoxyethanol, phosphate; ethanol, 2-butoxy-, phosphate (3:1); phosphoric acid, tributoxyethyl ester; tributyl cellosolve phosphate
Registered trade name(s)	Disflamoll TB; Celluphos 4; Phosflex 4[b]; Skydrol LD-4[b]	No data	Kronitex KP-140; KP 140; Phosflex T-bep
Chemical formula	$C_{12}H_{27}O_4P$	$C_{12}H_{27}O_4P$	$C_{18}H_{39}O_7P$
Chemical structure			
Identification numbers:			
CAS registry	126-73-8	126-71-6	78-51-3
RTECS[c]	TC7700000	No data	KJ9800000
EPA hazardous waste	No data	No data	No data
EPA/OPP pesticide Code	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	No data	No data	No data
HSDB	1678	No data	2564
EINECS	204-800-2	204-798-3	201-122-9
NCI	No data	No data	No data

Table 4-1. Chemical Identity of Selected Phosphate Ester Flame Retardants[a]

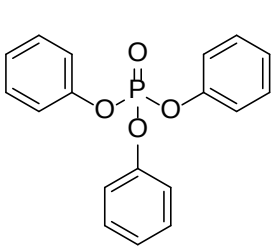
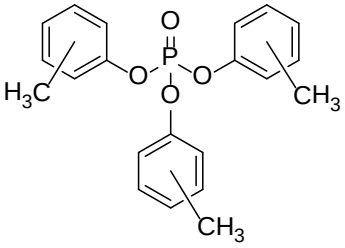
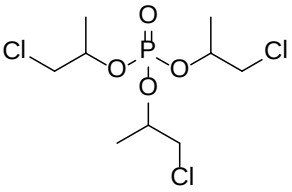
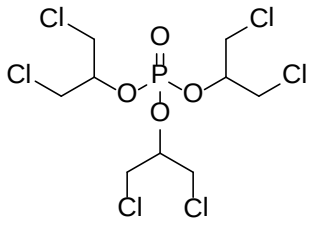
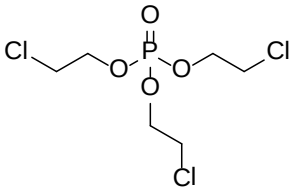
Characteristic	Triphenyl phosphate	Tricresyl phosphate	Tri-(2-chloroisopropyl) phosphate
Synonym(s)	TPP; phosphoric acid, triphenyl ester; triphenoxyphosphine oxide	TCP; phosphoric acid, tris(methylphenyl) ester; phosphoric acid, tritolyl ester; tris(methylphenyl) phosphate	TCPP; tris(1-chloro-2-propyl) phosphate; tris(2-chloroisopropyl) phosphate[d]; phosphoric acid, tris(2-chloro-1-methyl) ether[e]
Registered trade name(s)	Celluflex TPP; Disflamoll TP; Phosflex TPP	Kronitex TCP[b]; Phosflex 179A; Disflamoll TKP; Lindol; Celluflex 179C	Hostaflam OP 820; Amgard TMCP; Fyrol PFC[d]; Antiblaze 80[f]
Chemical formula	$C_{18}H_{15}O_4P$	$C_{21}H_{21}O_4P$	$C_9H_{18}Cl_3O_4P$
Chemical structure			
Identification numbers:			
CAS registry	115-86-6	1330-78-5	13674-84-5
RTECS[c]	TC8400000	TD0175000	TC9000000
EPA hazardous waste	No data	No data	No data
EPA/OPP Pesticide Code	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMDG shipping	IMO 9.0	UN 2574; IMO 6.1	No data
HSDB	2536	6774	No data
EINECS	204-112-2	215-548-8	237-158-7
NCI	No data	C61041	No data

Table 4-1. Chemical Identity of Selected Phosphate Ester Flame Retardants[a]

Characteristic	Tris(1,3-dichloro-2-propyl) phosphate	Tris(2-chloroethyl) phosphate
Synonym(s)	TDCP; tris(1,3-dichloroisopropyl) phosphate; tris(1-chloromethyl-2-chloroethyl)phosphate; 2-propanol, 1,3-dichloro-, phosphate (3:1)	TCEP; trichlorethyl phosphate; phosphoric acid; tris(2-chloroethyl)-ester; tri(2-chloroethyl) phosphate; ethanol, 2-chloro-, phosphate (3:1); tris(2-chloroethyl) orthophosphate
Registered trade name(s)	Fyrol FR-2; Antiblaze 195[f]	Antiblaze 100; Celluflex CEF; Disflamoll TCA; Fyrol CEF; Niax 3CF, Tolgard TCEP; Genomoll P; Hostaflam UP810; Levagard EP
Chemical formula	$C_9H_{15}Cl_6O_4P$	$C_6H_{12}Cl_3O_4P$
Chemical structure		
Identification numbers:		
CAS registry	13674-87-8	115-96-8
RTECS[c]	No data	KK2450000
EPA hazardous waste	No data	No data
EPA/OPP Pesticide Code	No data	No data
OHM/TADS	No data	No data
DOT/UN/NA/IMDG shipping	No data	UN: 3082[g]
HSDB	4364	2577
EINECS	237-159-2	204-118-5
NCI	No data	C60128

[a]All information obtained from HSDB 2009, 2011 and ChemIDplus 2009, 2011, except where noted.
[b]IPCS 1990,1991a, 2000b.
[c]RTECS 2009.
[d]Ashford 1994.
[e]Lewis 2000.
[f]Weil 2001.
[g]NIOSH 2007.

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/Intergovernmental Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Chemical Substances; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Physical and Chemical Properties of Selected Phosphate Ester Flame Retardants[a]

Property	Tributyl phosphate (TnBP)	Triisobutyl phosphate (TiBP)	Tris(2-butoxyethyl) phosphate (TBEP)
Molecular weight	266.31	266.31[c]	398.48
Physical description	Colorless to pale-yellow liquid	Clear, colorless, low viscosity liquid[c]	Slightly yellow, oily liquid
Melting point	-80 °C	No data	-70 °C
Boiling point	289 °C; decomposes[b]	264 °C[d]	215–228 °C at 4 mm Hg
Density	0.9727 g/cm^3 at 25 °C	0.9681 g/cm^3 at 20 °C[d]	1.020 g/cm^3 at 20 °C
Odor	Odorless	Specific odor[c]	Sweetish, butyl-like
Solubility:			
Water	0.28 g/L at 25 °C	Very soluble in water[c]; 0.05% in water[c] and 6.3% water in TnBP[c]	1.1 g/L at 25 °C
Organic solvent(s)	Soluble in diethyl ether, benzene, carbon disulfide; miscible with ethanol	Very soluble in benzene, ether, and ethanol[d]	Soluble in most organic liquids; soluble in mineral oil; insoluble or limited solubility in glycerol, glycols, certain amines
Other	Miscible with most solvents and diluents	No data	No data
Log K_{ow}	4.00	3.60 (estimated)[e]	3.75
Vapor pressure	1.13x10^{-3} mm Hg at 25 °C	0.0128 mm Hg at 25 °C (estimated)[e]	0.03 mm Hg at 150 °C
Autoignition temperature	>482 °C[b]	No data	No data
Flashpoint	146 °C	175 °C (Cleveland)[c]	223 °C
Flammability limits in air	Combustible	No data	Combustible
Conversion factors	1 ppm=10.89 mg/m^3[b]	No data	No data
Explosive limits	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Selected Phosphate Ester Flame Retardants[a]

Property	Triphenyl phosphate (TPP)	Tricresyl phosphate (TCP)	Tri-(2-chloroisopropyl) phosphate (TCPP)
Molecular weight	326.28	368.36	327.57
Physical Description	Colorless, crystalline powder; white platelets, crystals from absolute alcohol-ligroin, prisms from alcohol, needles from ether-ligroin	Colorless liquid[f]; Oily flame resistant liquid[g]	Colorless liquid[f]
Melting point	49–50 °C	-33 °C[h]	-40 °C
Boiling point	245 °C at 11 mm Hg	265 °C at 10 mm Hg[g]	>270 °C; gradually decomposes when heated over 200°C[f]
Density	1.2055 g/cm^3 at 50 °C	1.162 g/cm^3 at 25 °C	1.29 g/cm^3 at 25 °C[f]
Odor	Slightly aromatic odor resembling phenol	Odorless; very slightly aromatic[h]	Mild odor[f]
Solubility:			
Water	0.0019 g/L at 25 °C	0.00036 g/L at 25 °C	1.2 g/L at 25 °C
Organic solvents	Very soluble in carbon tetrachloride; soluble in alcohol, benzene, ether, chloroform and acetone; insoluble in petroleum	Miscible with all the common solvents and thinners	Soluble in most organic solvents; insoluble in water[f]
Other	Soluble in most lacquers, solvents thinners, and oils	Miscible with vegetable oil; Miscible with lindseed oil, china wood oil, castor oil[g]	No data
Log K_{ow}	4.59	5.11	2.59
Vapor pressure	6.28x10^{-6} mm Hg at 25 °C	6.00x10^{-7} mm Hg at 25 °C (extrapolated)[i]	2.02x10^{-5} mm Hg at 25 °C
Autoignition temperature	No data	No data	No data
Flashpoint	220 °C	257 °C[h]	No data
Flammability limits in air	Noncombustible	No data	No data
Conversion factors	1 ppm=13.32 mg/m^3	No data	No data
Explosive limits	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Selected Phosphate Ester Flame Retardants[a]

Property	Tris(1,3-dichloro-2-propyl) phosphate (TDCP)	Tris(2-chloroethyl) phosphate (TCEP)
Molecular weight	430.88	285.50
Physical Description	Viscous, clear liquid	Clear, transparent, Low viscosity liquid
Melting point	27 °C	-55 °C
Boiling point	236–237 °C at 5 mm Hg	330 °C at 1 atm
Density	1.48 g/cm^3 at 25 °C	1.425 g/cm^3 at 20 °C
Odor	Mild odor	Slight odor
Solubility:		
Water	7 mg/L at 24 °C	7.0 g/L (temperature not specified)
Organic solvents	Soluble in most organic solvents	Soluble in most organic solvents; soluble in carbon tetrachloride, alcohols, esters, ketones, and aromatic hydrocarbons; very slightly soluble in aliphatic hydrocarbons; insoluble in benzene
Other	No data	No data
Log K_{ow}	3.65	1.44
Vapor pressure	5.2 x10^{-2} mm Hg at 25 °C (estimated)[e]	6.125x10^{-2} mm Hg at 25 °C
Autoignition temperature	No data	1,115 °C
Flashpoint	252 °C	216 °C
Flammability limits in air	No data	Combustible
Conversion factors	No data	1 ppm=11.65 mg/m^3
Explosive limits	No data	No data

[a]All information obtained from HSDB 2009, 2011 and ChemIDplus 2009, 2011, except where noted.
[b]NIOSH 2005a.
[c]LANXESS 2005.
[d]Lide 2008.
[e]EPA 2009h.
[f]Ashford 1994.
[g]O'Neil et al. 2006.
[h]IPCS 1990.
[i]Boethling and Cooper 1985.