

Tri(2-chloroethyl) phosphate

Other names:	2-Chloro-ethanol phosphate (3:1)
	2-Chloroethanol phosphate
	3CF
	Celluflex
	Celluflex CEF
	Disflamoll TCA
	Ethanol, 2-chloro-, phosphate (3:1)
	Fyrol CEF
	Fyrol CF
	Genomoll P
	NCI-C60128
	NSC 3213
	Niax 3CF
	Niax Flame Retardant 3CF
	Phosphoric acid, tri-2-chloroethyl ester
	Phosphoric acid, tris(2-chloroethyl) ester
	TCEP
	Tri(«beta»-chloroethyl) phosphate
	Tri(Â«betaÂ»-chloroethyl) phosphate
	Trichlorethyl phosphate
	Trichloroethyl phosphate
	Tris(2-chloroethyl) orthophosphate
	Tris(2-chloroethyl) phosphate
	Tris(chloroethyl) phosphate
	Tris(«beta»-chloroethyl) phosphate
	Tris(Â«betaÂ»-chloroethyl) phosphate
	Tris-(2-chlorethyl)fosfat
Inchi:	InChI=1S/C6H12Cl3O4P/c7-1-4-11-14(10,12-5-2-8)13-6-3-9/h1-6H2
InchiKey:	HQUQLFOMPYWACS-UHFFFAOYSA-N
Formula:	C6H12Cl3O4P
SMILES:	O=P(OCCCI)(OCCCI)OCCCI
Mol. weight [g/mol]:	285.49
CAS:	115-96-8

Physical Properties

Property code	Value	Unit	Source
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log10ws	-3.32		Crippen Method
logp	2.861		Crippen Method
mcvol	176.060	ml/mol	McGowan Method
rinpol	1777.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	295.96		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1766.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	36.70	kJ/mol	369.00	NIST Webbook
pvap	4.80e-05	kPa	298.00	Determination of Vapor Pressures for Organophosphate Esters

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.19367e+01
Coeff. B	-4.41406e+03
Temperature range (K), min.	378.92
Temperature range (K), max.	666.25

Sources

Determination of Vapor Pressures for Organophosphate Esters: <https://www.doi.org/10.1021/je401026a>

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115968&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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