

Tris(2-chloropropyl) phosphate

Inchi:	InChI=1S/C9H18Cl3O4P/c1-7(10)4-14-17(13,15-5-8(2)11)16-6-9(3)12/h7-9H,4-6H2,1-3H3
InchiKey:	GTRSAMFYSUBAGN-UHFFFAOYSA-N
Formula:	C9H18Cl3O4P
SMILES:	CC(Cl)COP(=O)(OCC(C)Cl)OCC(C)Cl
Mol. weight [g/mol]:	327.57
CAS:	6145-73-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	4.026		Crippen Method
mcvol	218.330	ml/mol	McGowan Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6145739&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/10-535-6/Tris-2-chloropropyl-phosphate.pdf>

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