

1-Propanol, 2,3-dichloro-, phosphate (3:1)

Other names:	Propanol, 2,3-dichloro-, phosphate (3:1) Celluflex fr-2 FR 2 Phosphoric acid, tris(2,3-dichloropropyl) ester Tdcpp Tris-dichloropropylphosphate Tris(2,3-dichloropropyl)phosphate
Inchi:	InChI=1S/C9H15Cl6O4P/c10-1-7(13)4-17-20(16,18-5-8(14)2-11)19-6-9(15)3-12/h7-9H,1
InchiKey:	JZZBTMVTLBHJHL-UHFFFAOYSA-N
Formula:	C9H15Cl6O4P
SMILES:	O=P(OCC(Cl)CCl)(OCC(Cl)CCl)OCC(Cl)CCl
Mol. weight [g/mol]:	430.90
CAS:	78-43-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	4.683		Crippen Method
mcvol	255.050	ml/mol	McGowan Method
rinpol	2307.00		NIST Webbook
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rinpol	2307.00		NIST Webbook

Sources

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=C78433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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