

Phosphoric acid, bis[2-chloro-1-(chloromethyl)ethyl] 2,3-dichloropropyl ester

Other names: Bis(1,3-dichloro-2-propyl)-2,3-dichloro-1-propyl phosphate
Phosphoric acid, tris(1,3-dichloro-2-propyl) ester

bis[2-chloro-1-(chloromethyl)ethyl] 2,3-dichloropropyl phosphate

Inchi: InChI=1S/C9H15Cl6O4P/c10-1-7(15)6-17-20(16,18-8(2-11)3-12)19-9(4-13)5-14/h7-9H,1

InchiKey: PLUXGFREPRMQHY-UHFFFAOYSA-N

Formula: C9H15Cl6O4P

SMILES: O=P(OCC(Cl)CCl)(OC(CCl)CCl)OC(CCl)CCl

Mol. weight [g/mol]: 430.90

CAS: 68460-03-7

Physical Properties

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

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=C68460037&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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