

Phosphorodichloridothioic acid, o-propyl ester

Inchi:	InChI=1S/C3H7Cl2OPS/c1-2-3-6-7(4,5)8/h2-3H2,1H3
InchiKey:	BWTFGQULKVIPAH-UHFFFAOYSA-N
Formula:	C3H7Cl2OPS
SMILES:	CCCOP(=S)(Cl)Cl
Mol. weight [g/mol]:	193.03
CAS:	2523-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.27		Crippen Method
logp	3.115		Crippen Method
mcvol	120.290	ml/mol	McGowan Method

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=C2523968&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/16-809-6/Phosphorodichloridothioic-acid-o-propyl-ester.pdf>

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