

Phosphorodichloridothioic acid, s-ethyl ester

Inchi:	InChI=1S/C2H5Cl2OPS/c1-2-7-6(3,4)5/h2H2,1H3
InchiKey:	NZFDAHDTWVNSSI-UHFFFAOYSA-N
Formula:	C2H5Cl2OPS
SMILES:	CCSP(=O)(Cl)Cl
Mol. weight [g/mol]:	179.00
CAS:	1486-40-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.325		Crippen Method
mcvol	106.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1486404&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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