

O-Methyl S-2-diisopropylaminoethyl ethylphosphonothiolate

Other names:	Ethyl-phosphonothioic acid, S-(2-diisopropylamino-ethyl) O-methyl ester Phosphonothioic acid, ethyl-, S-[2-[bis(1-methylethyl)amino]ethyl] O-methyl ester Ethyl-phosphonothioic acid S-(2-diisopropylamino-ethyl) ester O-methyl ester
Inchi:	InChI=1S/C11H26NO2PS/c1-7-15(13,14-6)16-9-8-12(10(2)3)11(4)5/h10-11H,7-9H2,1-6H
InchiKey:	AVIWKFSOYDOCNU-UHFFFAOYSA-N
Formula:	C11H26NO2PS
SMILES:	CCP(=O)(OC)SCCN(C(C)C)C(C)C
Mol. weight [g/mol]:	267.37
CAS:	162085-94-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.698		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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