

O-Isopropyl S-2-diethylaminoethyl ethylphosphonothiolate

Other names:	Ethyl-phosphonothioic acid S-(2-diethylamino-ethyl) O-isopropyl ester Phosphonothioic acid, ethyl-, S-[2-(diethylamino)ethyl] O-(1-methylethyl) ester Ethyl-phosphonothioic acid S-(2-diethylamino-ethyl) ester O-isopropyl ester
Inchi:	InChI=1S/C11H26NO2PS/c1-6-12(7-2)9-10-16-15(13,8-3)14-11(4)5/h11H,6-10H2,1-5H3
InchiKey:	WKTMOYXLDZRCF-UHFFFAOYSA-N
Formula:	C11H26NO2PS
SMILES:	CCN(CC)CCSP(=O)(CC)OC(C)C
Mol. weight [g/mol]:	267.37
CAS:	162085-93-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.699		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook

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=C162085930&Units=SI

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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