

O-Isopropyl S-2-diisopropylaminoethyl ethylphosphonothiolate

Other names:	Ethyl-phosphonothioic acid S-(2-diisopropylamino-ethyl) ester O-isopropyl ester
Inchi:	InChI=1S/C13H30NO2PS/c1-8-17(15,16-13(6)7)18-10-9-14(11(2)3)12(4)5/h11-13H,8-10
InchiKey:	DGZWREVCJRZEFR-UHFFFAOYSA-N
Formula:	C13H30NO2PS
SMILES:	CCP(=O)(OC(C)C)SCCN(C(C)C)C(C)C
Mol. weight [g/mol]:	295.42
CAS:	162085-95-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	4.476		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
rinpol	1789.00		NIST Webbook
rinpol	1789.30		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1789.30		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085952&Units=SI
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

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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