S-Ethyl S-(2-diisopropylaminoethyl) methylphosphonodithioate

Other names: S-Ethyl-S-[2-(diisopropylamino)ethyl]methylphosphonothiodithiolate
S-Ethyl S-[2-(diisopropylamino)ethyl]methylphosphonothiolate
Methyldithiophosphonic acid, S-ethyl, S-(2-diisopropylaminoethyl) ester

Inchi: InChI=1S/C11H26NOPS2/c1-7-15-14(6,13)16-9-8-12(10(2)3)11(4)5/h10-11H,7-9H2,1-6H

InchiKey: WALRJEDABGCYFW-UHFFFAOYSA-N

Formula: C11H26NOPS2

SMILES: CCSP(C)(=O)SCCN(C(C)C)C(C)C

Mol. weight [g/mol]: 283.43

CAS: 110501-55-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	4.414		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
rinpol	1760.00		NIST Webbook
rinpol	1793.10		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1793.10		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110501558&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