O-Methyl S-2-diethylaminoethyl ethylphosphonothiolate

Other names: Ethyl-phosphonothioic acid S-(2-diethylamino-ethyl) ester O-methyl ester
Inchi: InChI=1S/C9H22NO2PS/c1-5-10(6-2)8-9-14-13(11,7-3)12-4/h5-9H2,1-4H3
InchiKey: MVKMTTUVZUUMGU-UHFFFAOYSA-N
Formula: C9H22NO2PS
SMILES: CCN(CC)CCSP(=O)(CC)OC
Mol. weight [g/mol]: 239.31
CAS: 170800-77-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.921		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
rinpol	1621.70		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1621.70		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C170800778&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