O-Ethyl S-2-dimethylaminoethyl ethylphosphonothiolate

Other names: Ethyl-phosphonothioic acid S-(2-dimethylamino-ethyl) ester O-ethyl ester
Inchi: InChI=1S/C8H20NO2PS/c1-5-11-12(10,6-2)13-8-7-9(3)4/h5-8H2,1-4H3
InchiKey: LLMAYCPOBKHQIP-UHFFFAOYSA-N
Formula: C8H20NO2PS
SMILES: CCOP(=O)(CC)SCCN(C)C
Mol. weight [g/mol]: 225.29
CAS: 98543-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.531		Crippen Method
mcvol	182.110	ml/mol	McGowan Method
rinpol	1521.70		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1521.70		NIST Webbook
rinpol	1522.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98543250&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