O-Ethyl S-2-diethylaminoethyl ethylphosphonothiolate

Other names: S-[2-(Diethylamino)ethyl] o-ethyl ethylphosphonothioate
Ethyl-phosphonothioic acid S-(2-diethylamino-ethyl) ester O-ethyl ester
VE

Inchi: InChI=1S/C10H24NO2PS/c1-5-11(6-2)9-10-15-14(12,8-4)13-7-3/h5-10H2,1-4H3

InchiKey: QXRUNSUMQBTCQS-UHFFFAOYSA-N

Formula: C10H24NO2PS

SMILES: CCOP(=O)(CC)SCCN(CC)CC

Mol. weight [g/mol]: 253.34

CAS: 21738-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	3.311		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
rinpol	1622.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1670.90		NIST Webbook
rinpol	1671.00		NIST Webbook

Sources

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=C21738250&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices