O-Ethyl S-2-dimethylaminoethyl methylphosphonothiolate

Other names: S-[2-(Dimethylamino)ethyl] O-ethyl methylphosphonothioate
Methyl-phosphonothioic acid S-(2-dimethylamino-ethyl) ester O-ethyl ester
Medemo

Inchi: InChI=1S/C7H18NO2PS/c1-5-10-11(4,9)12-7-6-8(2)3/h5-7H2,1-4H3

InchiKey: PKDYQTANBZBIRM-UHFFFAOYSA-N

Formula: C7H18NO2PS

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

Mol. weight [g/mol]: 211.26

CAS: 20820-80-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	2.141		Crippen Method
mcvol	168.020	ml/mol	McGowan Method
rinpol	1442.00		NIST Webbook
rinpol	1442.50		NIST Webbook
rinpol	1442.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20820808&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