

O-Isopropyl S-2-dimethylaminoethyl ethylphosphonothiolate

Other names: Ethyl-phosphonothioic acid S-(2-dimethylamino-ethyl) ester O-isopropyl ester
Inchi: InChI=1S/C9H22NO2PS/c1-6-13(11,12-9(2)3)14-8-7-10(4)5/h9H,6-8H2,1-5H3
InchiKey: BIMXZYDFIXDYDT-UHFFFAOYSA-N
Formula: C9H22NO2PS
SMILES: CCP(=O)(OC(C)C)SCCN(C)C
Mol. weight [g/mol]: 239.31
CAS: 162085-92-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.919		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
rinpol	1532.40		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1532.00		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=C162085929&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

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