

Methylthophosphonic acid, O-isobutyl S-(2-diethylaminoethyl) ester

Inchi: InChI=1S/C12H27O2PS/c1-6-12(7-2)8-9-16-15(5,13)14-10-11(3)4/h11-12H,6-10H2,1-5H
InchiKey: SKOSVDAPQCDRDB-UHFFFAOYSA-N
Formula: C12H27O2PS
SMILES: CCC(CC)CCSP(C)(=O)OCC(C)C
Mol. weight [g/mol]: 266.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	5.041		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
rinpol	1675.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1675.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R559558&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

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