

Methyldithosphonic acid, S-isobutyl S-(2-diethylaminoethyl) ester

Inchi: InChI=1S/C8H20NOPS2/c1-5-9(6-2)7-8-13-11(3,10)12-4/h5-8H2,1-4H3
InchiKey: RIFTXTUCDJTCNY-UHFFFAOYSA-N
Formula: C8H20NOPS2
SMILES: CCN(CC)CCSP(C)(=O)SC
Mol. weight [g/mol]: 241.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	3.247		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
rinpol	1768.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1768.00		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=R559523&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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