Methylthiophosphonic acid, O-isobutyl, S-2-(2-(diethylaminoethylthio)ethyl) ester

Inchi: InChI=1S/C13H30NO2PS2/c1-6-14(7-2)8-9-18-10-11-19-17(5,15)16-12-13(3)4/h13H,6-1

InchiKey: GHZZDPPFZNDIER-UHFFFAOYSA-N

Formula: C13H30NO2PS2

SMILES: CCN(CC)CCSCCSP(C)(=O)OCC(C)C

Mol. weight [g/mol]: 327.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	4.290		Crippen Method
mcvol	268.910	ml/mol	McGowan Method
rinpol	2128.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R334913&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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