Methylthiophosphonic acid, O-isobutyl, S-(2-(2-(2-diethylaminoethylthio)ethylthio)ethylthi

Other names: Methylthiophosphonic acid, O-isobutyl S-{2-[2-(2-diethylaminoethylthio)ethylthio]ethyl} ester

Inchi: InChI=1S/C15H34NO2PS3/c1-6-16(7-2)8-9-20-10-11-21-12-13-22-19(5,17)18-14-15(3)4

InchiKey: PDCSQNAEOZNCPZ-UHFFFAOYSA-N

Formula: C15H34NO2PS3

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

Mol. weight [g/mol]: 387.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	5.023		Crippen Method
mcvol	313.440	ml/mol	McGowan Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook
rinpol	2636.00		NIST Webbook
rinpol	2648.00		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=R338544&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