

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

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

Latest version available from:

<https://www.cheméo.com/cid/79-316-4/Methylthiophosphonic-acid-O-isobutyl-S-2-2-2-diethylaminoethylthio-ethylthio->

Generated by Cheméo on 2025-12-06 01:00:48.404555294 +0000 UTC m=+4731045.934595960.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.