

Methylphosphonic acid, methyl 2-(diethylamino)ethyl ester

Inchi: InChI=1S/C8H20NO3P/c1-5-9(6-2)7-8-12-13(4,10)11-3/h5-8H2,1-4H3
InchiKey: TYPZPSKRZIRPIQ-UHFFFAOYSA-N
Formula: C8H20NO3P
SMILES: CCN(CC)CCOP(C)(=O)OC
Mol. weight [g/mol]: 209.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	1.814		Crippen Method
mcvol	171.630	ml/mol	McGowan Method
rinsol	1424.00		NIST Webbook
rinsol	1424.00		NIST Webbook
rinsol	1446.00		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=R403722&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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