

Methylthiophosphonic acid, S-(2-diethylaminoethyl) ester

Inchi: InChI=1S/C7H18NO2PS/c1-4-8(5-2)6-7-12-11(3,9)10/h4-7H2,1-3H3,(H,9,10)
InchiKey: VDVPFYBCCCESMG-UHFFFAOYSA-N
Formula: C7H18NO2PS
SMILES: CCN(CC)CCSP(C)(=O)O
Mol. weight [g/mol]: 211.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	1.877		Crippen Method
mcvol	168.020	ml/mol	McGowan Method
rinsol	1424.00		NIST Webbook
rinsol	1424.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R334933&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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