

N,n-dimethyl-p-methyl phosphonamidic acid, n-pentyl ester

Inchi: InChI=1S/C8H20NO2P/c1-5-6-7-8-11-12(4,10)9(2)3/h5-8H2,1-4H3
InchiKey: QGJLHUMSQHTIRU-UHFFFAOYSA-N
Formula: C8H20NO2P
SMILES: CCCCCOP(C)(=O)N(C)C
Mol. weight [g/mol]: 193.22
CAS: 114328-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	2.578		Crippen Method
mcvol	165.760	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C114328802&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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