

Phosphonic acid, methyl-, 2-[bis(1-methylethyl)amino]ethyl ethyl ester

Other names:

Methylphosphonic acid (2-(bis(1-methylethyl)amino)ethyl) ethyl ester

Ethyl 2-(diisopropylamino)ethyl methylphosphonate

Phosphonic acid, methyl, ethyl-2-(diisopropylaminoethyl) ester

O-Ethyl-O'-(2-diisopropylaminoethyl)methylphosphonate

Methylphosphonic acid, ethyl 2-diisopropylaminoethyl ester

Inchi:

InChI=1S/C11H26NO3P/c1-7-14-16(6,13)15-9-8-12(10(2)3)11(4)5/h10-11H,7-9H2,1-6H3

InchiKey:

IEMIPTMSCIDZLN-UHFFFAOYSA-N

Formula:

C11H26NO3P

SMILES:

CCOP(C)(=O)OCCN(C(C)C)C(C)C

Mol. weight [g/mol]:

251.30

CAS:

71840-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	2.981		Crippen Method
mcvol	213.900	ml/mol	McGowan Method
rinpol	1530.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C71840261&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/23-114-9/Phosphonic-acid-methyl-2-bis-1-methylethyl-amino-ethyl-ethyl-ester.pdf>

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