O-(2-DIISOPROPYLAMINOETHYL) O'-ETHYL METHYLPHOSPHONATE

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]: 251.31

Physical Properties

Property code	Value	Unit	Source
hvap	71.48	kJ/mol	Cheméo Relay (1.0)
logp	2.981		Crippen Method
mcvol	213.900	ml/mol	McGowan Method
rinpol	1530.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71840261&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

hvap: Enthalpy of vaporization at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices