

PENTAMETHYLPHOSPHONIC DIAMIDE

Other names:	Phosphonic diamide, pentamethyl- N,N,N',N'-Tetramethylmethylphosphonamide Phosphorodiamidous acid, tetramethyl-, methyl ester N,N,N',N'-Tetramethyl methanephosphorodiamide
Inchi:	InChI=1S/C5H15N2OP/c1-6(2)9(5,8)7(3)4/h1-5H3
InchiKey:	YRWJRJCUCZYGLPN-UHFFFAOYSA-N
Formula:	C5H15N2OP
SMILES:	CN(C)P(C)(=O)N(C)C
Mol. weight [g/mol]:	150.16

Physical Properties

Property code	Value	Unit	Source
affp	951.30	kJ/mol	NIST Webbook
basg	918.90	kJ/mol	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
logp	0.933		Crippen Method
mccvol	127.600	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2511173&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

affp: Proton affinity

basg:	Gas basicity
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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