

PHOSPHORIC TRIAMIDE, PENTAMETHYL-

Other names:	ENT 51295 Pentamethylphosphoric triamide Pentamethylphosphoramidate
Inchi:	InChI=1S/C5H16N3OP/c1-6-10(9,7(2)3)8(4)5/h1-5H3,(H,6,9)
InchiKey:	JSJBYUNWLNWERF-UHFFFAOYSA-N
Formula:	C5H16N3OP
SMILES:	CNP(=O)(N(C)C)N(C)C
Mol. weight [g/mol]:	165.18

Physical Properties

Property code	Value	Unit	Source
ie	8.55 ± 0.05	eV	NIST Webbook
logp	0.437		Crippen Method
mcvol	137.580	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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10159463&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/72-984-0/PHOSPHORIC-TRIAMIDE-PENTAMETHYL.pdf>

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