

1,4,8,11-Tetraazacyclotetradecane, 1,4,8,11-tetramethyl-

Other names: 1,4,8,11-Tetramethyl-1,4,8,11-tetraazacyclotetradecane

Tetramethylcyclam

Inchi: InChI=1S/C14H32N4/c1-15-7-5-8-17(3)13-14-18(4)10-6-9-16(2)12-11-15/h5-14H2,1-4H3

InchiKey: HRFJEOWVAGSJNW-UHFFFAOYSA-N

Formula: C14H32N4

SMILES: CN1CCCN(C)CCN(C)CCN(C)CC1

Mol. weight [g/mol]: 256.43

CAS: 41203-22-9

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
log10ws	0.14		Crippen Method
logp	0.507		Crippen Method
mcvol	237.180	ml/mol	McGowan Method

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C41203229&Units=SI>

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

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

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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