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)CCCN(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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41203229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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