

1,2,3,4,6,7,8,9,10,11-Decahydro-4a,12-diaza-cycloocta-b-naphthalen-5-one

Inchi:	InChI=1S/C14H20N2O/c17-14-11-7-3-1-2-4-8-12(11)15-13-9-5-6-10-16(13)14/h1-10H2
InchiKey:	QFUPHXFAXNXJOO-UHFFFAOYSA-N
Formula:	C14H20N2O
SMILES:	O=c1c2c(nc3n1CCCC3)CCCCC2
Mol. weight [g/mol]:	232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	2.239		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R318233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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