

1,2,3,5,6,7,8,9-Octahydro-3a,10-diaza-cyclohepta[1

Inchi:	InChI=1S/C12H16N2O/c15-12-9-5-2-1-3-6-10(9)13-11-7-4-8-14(11)12/h1-8H2
InchiKey:	FICCMFSHBVQZHA-UHFFFAOYSA-N
Formula:	C12H16N2O
SMILES:	O=c1c2c(nc3n1CCC3)CCCCC2
Mol. weight [g/mol]:	204.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	1.458		Crippen Method
mcvol	160.290	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R318273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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