

2,3,5,6,7,8-Hexahydro-1H-4,8a-diaza-cyclopenta[b]

Other names:	2,3,5,6,7,8-Hexahydro-1H-4,8a-diaza-cyclopenta[b]naphthalen-9-one
Inchi:	InChI=1S/C11H14N2O/c14-11-8-4-3-5-9(8)12-10-6-1-2-7-13(10)11/h1-7H2
InchiKey:	GMFURYYNPXKBGY-UHFFFAOYSA-N
Formula:	C11H14N2O
SMILES:	O=c1c2c(nc3n1CCCC3)CCC2
Mol. weight [g/mol]:	190.25

Physical Properties

Property code	Value	Unit	Source
logp	1.068		Crippen Method
mcvol	146.200	ml/mol	McGowan Method
rinpol	1961.00		NIST Webbook
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rinpol	1961.00		NIST Webbook

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=R119789&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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