6,7,8,9,10,11-Hexahydro-5,11a-diaza-cycloocta[b]naphthalen-12-one

Inchi: InChI=1S/C14H16N2O/c17-14-11-7-4-5-8-12(11)15-13-9-3-1-2-6-10-16(13)14/h4-5,7-8H

InchiKey: RJDGOLWDHKFBOF-UHFFFAOYSA-N

Formula: C14H16N2O

SMILES: O=c1c2ccccc2nc2n1CCCCCC2

Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	2.513		Crippen Method
mcvol	179.870	ml/mol	McGowan Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R318397&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.