6,7,8,9,10,11-Hexahydro-4a,12-diaza-cycloocta[b]n

Inchi: InChI=1S/C14H16N2O/c17-14-11-7-3-1-2-4-8-12(11)15-13-9-5-6-10-16(13)14/h5-6,9-10H
InchiKey: SNXFGZHGSIBQMQ-UHFFFAOYSA-N
Formula: C14H16N2O
SMILES: O=c1c2c(nc3ccccn13)CCCCCC2
Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	2.353		Crippen Method
mcvol	179.870	ml/mol	McGowan Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		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=R318382&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.