2,3,4,5,7,8,9,10,11,12-Decahydro-1H-5a,13-diaza-c

Inchi: InChI=1S/C15H22N2O/c18-15-12-8-4-1-2-5-9-13(12)16-14-10-6-3-7-11-17(14)15/h1-11H
InchiKey: XXXSHXCCZQCCLR-UHFFFAOYSA-N
Formula: C15H22N2O
SMILES: O=c1c2c(nc3n1CCCCC3)CCCCCC2
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.629		Crippen Method
mcvol	202.560	ml/mol	McGowan Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		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=R318322&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.