1,2,3,4,6,7,8,9,10,11-Decahydro-5,11a-diaza-cyclo

Inchi: InChI=1S/C14H20N2O/c17-14-11-7-4-5-8-12(11)15-13-9-3-1-2-6-10-16(13)14/h1-10H2
InchiKey: WCFODMJXNQITOI-UHFFFAOYSA-N
Formula: C14H20N2O
SMILES: O=c1c2c(nc3n1CCCCCC3)CCCC2
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	2.239		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
rinpol	2165.00		NIST Webbook

Sources

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=R318248&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:
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