Dihydrocytisine

Inchi: InChI=1S/C11H16N2O/c14-11-3-1-2-10-9-4-8(5-12-6-9)7-13(10)11/h1,3,8-10,12H,2,4-7H
InchiKey: KSXAIQGMVVISIG-UHFFFAOYSA-N
Formula: C11H16N2O
SMILES: O=C1C=CCC2C3CNCC(C3)CN12
Mol. weight [g/mol]: 192.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Crippen Method
logp	0.383		Crippen Method
mcvol	150.500	ml/mol	McGowan Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		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=R205424&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.