11-Allylcytisine

Inchi: InChI=1S/C14H22N2O/c1-2-6-15-8-11-7-12(10-15)13-4-3-5-14(17)16(13)9-11/h2,11-13H
InchiKey: WBLAJWUPDFINPQ-UHFFFAOYSA-N
Formula: C14H22N2O
SMILES: C=CCN1CC2CC(C1)C1CCCC(=O)N1C2
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	1.505		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
rinpol	2250.00		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=R308439&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