

11-Allylcytisine

Inchi: InChI=1S/C14H18N2O/c1-2-6-15-8-11-7-12(10-15)13-4-3-5-14(17)16(13)9-11/h2-5,11-12
InchiKey: MKBCSSZRYRIMHK-UHFFFAOYSA-N
Formula: C14H18N2O
SMILES: C=CCN1CC2CC(C1)c1cccc(=O)n1C2
Mol. weight [g/mol]: 230.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	1.453		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
rinpol	2245.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2262.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R261122&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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