

# 11-Allylcytisine

<b>Inchi:</b>	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
<b>InchiKey:</b>	WBLAJWUPDFINPQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H22N2O
<b>SMILES:</b>	C=CCN1CC2CC(C1)C1CCCC(=O)N1C2
<b>Mol. weight [g/mol]:</b>	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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R308439&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308439&amp;Units=SI</a>

## Legend

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

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