

# N-acetylcytisine

<b>Other names:</b>	N-Acetylytisine
<b>Inchi:</b>	InChI=1S/C13H16N2O2/c1-9(16)14-6-10-5-11(8-14)12-3-2-4-13(17)15(12)7-10/h2-4,10-
<b>InchiKey:</b>	WCRIKJOQMRFVPX-UHFFFAOYSA-N
<b>Formula:</b>	C13H16N2O2
<b>SMILES:</b>	CC(=O)N1CC2CC(C1)c1cccc(=O)n1C2
<b>Mol. weight [g/mol]:</b>	232.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	0.814		Crippen Method
mcvol	175.950	ml/mol	McGowan Method
rinpol	2320.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2323.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2320.00		NIST Webbook

## Sources

<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=R261177&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R261177&amp;Units=SI</a>
<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>

# 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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