

# N-Methylammodendrine

**Inchi:** InChI=1S/C13H22N2O/c1-11(16)15-9-5-6-12(10-15)13-7-3-4-8-14(13)2/h10,13H,3-9H2,1  
**InchiKey:** SWGUPFWFYUMIGH-UHFFFAOYSA-N  
**Formula:** C13H22N2O  
**SMILES:** CC(=O)N1C=C(C2CCCCN2C)CCC1  
**Mol. weight [g/mol]:** 222.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	1.997		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
rinpol	1835.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1835.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R264329&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

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