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/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=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