Dehydroammodendrine

Inchi: InChI=1S/C12H18N2O/c1-10(15)14-8-4-5-11(9-14)12-6-2-3-7-13-12/h7,9,12H,2-6,8H2,1
InchiKey: QNIAXHGFFZVMHW-UHFFFAOYSA-N
Formula: C12H18N2O
SMILES: CC(=O)N1C=C(C2CCCC=N2)CCC1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	2.136		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
rinpol	1932.00		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=R264121&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