

Dihydroammოდendrine

Inchi: InChI=1S/C12H22N2O/c1-10(15)14-8-4-5-11(9-14)12-6-2-3-7-13-12/h11-13H,2-9H2,1H3
InchiKey: BQZMRUJJCKKJNX-UHFFFAOYSA-N
Formula: C12H22N2O
SMILES: CC(=O)N1CCCC(C2CCCCN2)C1
Mol. weight [g/mol]: 210.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.387		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
rinpol	1850.00		NIST Webbook
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Sources

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=R261197&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/25-242-5/Dihydroammოდendrine.pdf>

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