

9-Angeloyltrachelanthamidine

Inchi: InChI=1S/C13H21NO2/c1-3-10(2)13(15)16-9-11-6-8-14-7-4-5-12(11)14/h3,11-12H,4-9H2
InchiKey: NWPCVTQQFKZNSF-VZAOXQLQSA-N
Formula: C13H21NO2
SMILES: CC=C(C)C(=O)OCC1CCN2CCCC12
Mol. weight [g/mol]: 223.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.980		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R227939&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

Latest version available from:

<https://www.chemeo.com/cid/11-289-9/9-Angeloyltrachelanthamidine.pdf>

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