

Acetylepilupinine

Inchi: InChI=1S/C12H21NO2/c1-10(14)15-9-11-5-4-8-13-7-3-2-6-12(11)13/h11-12H,2-9H2,1H3
InchiKey: WRCNAOJPCHQUCI-PXYINDEMSA-N
Formula: C12H21NO2
SMILES: CC(=O)OCC1CCCN2CCCCC12
Mol. weight [g/mol]: 211.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	1.814		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
rinpol	1513.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R261142&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/55-594-2/Acetylepilupinine.pdf>

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