

N-Propionylnorloline

Inchi: InChI=1S/C11H18N2O/c1-2-9(14)12-10-8-5-7-3-4-13(6-8)11(7)10/h7-8,10-11H,2-6H2,1H
InchiKey: RRMMYRUWUOQJNI-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: CCC(=O)NC1C2CC3CCN(C2)C31
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	0.605		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
rinpole	1660.00		NIST Webbook

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=R274341&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/46-733-7/N-Propionylnorloline.pdf>

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