

N-AcetylNorloline

Inchi: InChI=1S/C9H14N2O2/c1-5(12)10-8-7-4-11-3-2-6(13-7)9(8)11/h6-9H,2-4H2,1H3,(H,10,11)
InchiKey: BWGXNGORZPWYGZ-OBCZXFEGSA-N
Formula: C9H14N2O2
SMILES: CC(=O)NC1C2CN3CCC(O2)C13
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.34		Crippen Method
logp	-0.654		Crippen Method
mcvol	132.490	ml/mol	McGowan Method
rinpole	1575.00		NIST Webbook
rinpole	1575.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R268356&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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