

Loline

Inchi: InChI=1S/C8H14N2O/c1-9-7-6-4-10-3-2-5(11-6)8(7)10/h5-9H,2-4H2,1H3/t5-,6+,7-,8?/m0
InchiKey: OPMNROCQHKJDAQ-SZVWITLZSA-N
Formula: C8H14N2O
SMILES: CNC1C2CN3CCC(O2)C13
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.15		Crippen Method
logp	-0.570		Crippen Method
mcvol	116.830	ml/mol	McGowan Method
rinpol	1252.00		NIST Webbook
rinpol	1250.00		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=R268316&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/35-304-5/Loline.pdf>

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