

4«beta»-hydroxylupinine

Inchi: InChI=1S/C10H19NO2/c12-7-8-4-5-10(13)11-6-2-1-3-9(8)11/h8-10,12-13H,1-7H2/t8-,9+,
InchiKey: XJGGJDSGTDKLPJ-IVZWLZJFSA-N
Formula: C10H19NO2
SMILES: OCC1CCC(O)N2CCCCC12
Mol. weight [g/mol]: 185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	0.562		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
rinpol	1605.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R261335&Units=SI>
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>

Legend

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

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