

3«beta»-hydroxyroboidine

Inchi: InChI=1S/C20H27N3O4/c24-18-4-3-16-12-8-13(11-23(16)19(18)25)17-9-14(5-7-22(17)10-20)21-6-2
InchiKey: KJNJUSLRLXSFGC-WANSGLISSA-N
Formula: C20H27N3O4
SMILES: O=C(OC1CCN2CC3CC(CN4C(=O)C(O)CCC34)C2C1)c1ccc[nH]1
Mol. weight [g/mol]: 373.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	0.524		Crippen Method
mcvol	274.580	ml/mol	McGowan Method
rinpol	3160.00		NIST Webbook
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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=R322113&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

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<https://www.chemeo.com/cid/33-948-3/3-beta-hydroxyroboidine.pdf>

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