

13-Hydroxymultiflorine

Inchi: InChI=1S/C15H24N2O2/c18-12-1-3-16-8-10-5-11(14(16)6-12)9-17-4-2-13(19)7-15(10)17
InchiKey: XSWCLXUQXOJCGT-UHFFFAOYSA-N
Formula: C15H24N2O2
SMILES: O=C1CCN2CC3CC(CN4CCC(O)CC34)C2C1
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	0.495		Crippen Method
mcvol	206.170	ml/mol	McGowan Method
rinpol	2570.00		NIST Webbook
rinpol	2558.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R263955&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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