

13«alpha»-Hydroxymultiflorine

Inchi:	InChI=1S/C15H22N2O2/c18-12-1-3-16-8-10-5-11(14(16)6-12)9-17-4-2-13(19)7-15(10)17
InchiKey:	WADQXAAHRPKPQW-WAMZBAIXSA-N
Formula:	C15H22N2O2
SMILES:	O=C1C=CN2CC3CC(CN4CCC(O)CC34)C2C1
Mol. weight [g/mol]:	262.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.56		Crippen Method
logp	0.619		Crippen Method
mcvol	201.870	ml/mol	McGowan Method
rinpol	2566.00		NIST Webbook
rinpol	2566.00		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=R557012&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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