

4«beta»-Hydroxyepilupinine

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-,1-
InchiKey:	XJGGJDSGTDKLPJ-LPEHRKFASA-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
rinpole	1605.00		NIST Webbook

Sources

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=R261182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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