

# 13-Hydroxy-17-oxolupanine

**Inchi:** InChI=1S/C15H22N2O3/c18-9-4-5-12-11-8-17-13(2-1-3-14(17)19)10(15(11)20)7-16(12)6  
**InchiKey:** GDHIGJBIQZNHST-UHFFFAOYSA-N  
**Formula:** C15H22N2O3  
**SMILES:** O=C1C2CN3C(=O)CCCC3C1CN1CC(O)CCC21  
**Mol. weight [g/mol]:** 278.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.99		Crippen Method
logp	0.022		Crippen Method
mcvol	207.740	ml/mol	McGowan Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R263940&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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