

# 13-Acetyloxy-lupanine

**Other names:** 13-acetoxylupanine  
**Inchi:** InChI=1S/C17H26N2O3/c1-11(20)22-15-4-6-18-13(9-15)7-12-8-14(18)10-16-17(21)3-2-5  
**InchiKey:** SFMOQALRSJSJBL-UHFFFAOYSA-N  
**Formula:** C17H26N2O3  
**SMILES:** CC(=O)OC1CCN2C(C1)CC1CC2CC2C(=O)CCCN12  
**Mol. weight [g/mol]:** 306.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	1.351		Crippen Method
mcvol	235.920	ml/mol	McGowan Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R261246&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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