

# 13-Angeloyloxy-17-oxolupanine

**Inchi:** InChI=1S/C20H28N2O4/c1-3-12(2)20(25)26-13-7-8-16-15-11-22-17(5-4-6-18(22)23)14(1)  
**InchiKey:** JMBDSDRKAFJRFY-BASWHVEKSA-N  
**Formula:** C20H28N2O4  
**SMILES:** CC=C(C)C(=O)OC1CCC2C3CN4C(=O)CCCC4C(CN2C1)C3=O  
**Mol. weight [g/mol]:** 360.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	1.539		Crippen Method
mcvol	275.460	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263886&Units=SI>  
**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>

## 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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