

# 13«beta»-Tygloyloxylupanine

**Inchi:** InChI=1S/C20H30N2O3/c1-3-13(2)20(24)25-16-7-8-21-11-14-9-15(18(21)10-16)12-22-17  
**InchiKey:** UPVPJQNTGLTBPC-PFRCDYALSA-N  
**Formula:** C20H30N2O3  
**SMILES:** CC=C(C)C(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1  
**Mol. weight [g/mol]:** 346.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.360		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
rinsol	2850.00		NIST Webbook
rinsol	2850.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=R557052&Units=SI>

## Legend

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

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