

# 7-Angeloylplatynecine

**Inchi:** InChI=1S/C13H21NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h3,10-12,15H  
**InchiKey:** JVBOUYIVPAHNGB-ZRNSCVGCSA-N  
**Formula:** C13H21NO3  
**SMILES:** CC=C(C)C(=O)OC1CCN2CCC(CO)C12  
**Mol. weight [g/mol]:** 239.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	0.951		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
rinpole	1818.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178337&Units=SI>  
**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>

## 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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