

# 7,9-Disenecioylplatynecine

**Inchi:** InChI=1S/C18H27NO4/c1-12(2)9-16(20)22-11-14-5-7-19-8-6-15(18(14)19)23-17(21)10-1  
**InchiKey:** CUJDQFVONFREPO-MPGHIAIKSA-N  
**Formula:** C18H27NO4  
**SMILES:** CC(C)=CC(=O)OCC1CCN2CCC(OC(=O)C=C(C)C)C12  
**Mol. weight [g/mol]:** 321.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	2.468		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
rinpol	2230.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2230.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177963&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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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