

# 9-Tigloylplatynecine

**Inchi:** InChI=1S/C13H21NO3/c1-3-9(2)13(16)17-8-10-4-6-14-7-5-11(15)12(10)14/h3,10-12,15H  
**InchiKey:** FOWFFDPFIJUTGG-GVOVMLPNSA-N  
**Formula:** C13H21NO3  
**SMILES:** CC=C(C)C(=O)OCC1CCN2CCC(O)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
rinpol	1895.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook

## Sources

**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=R178075&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/37-426-8/9-Tigloylplatynecine.pdf>

Generated by Cheméo on 2024-04-23 09:57:49.523553454 +0000 UTC m=+16155518.444130766.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.