

# 3-Hydroxy-6-Tigloyloxytropane

**Inchi:** InChI=1S/C13H21NO3/c1-4-8(2)13(16)17-12-6-9-5-10(15)7-11(12)14(9)3/h4,9-12,15H,5  
**InchiKey:** FSTVJNLNEVDORU-XBXARRHUSA-N  
**Formula:** C13H21NO3  
**SMILES:** CC=C(C)C(=O)OC1CC2CC(O)CC1N2C  
**Mol. weight [g/mol]:** 239.31  
**CAS:** 110024-55-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	1.092		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
rinpol	1836.00		NIST Webbook
rinpol	1905.80		NIST Webbook
rinpol	1839.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C110024550&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)

## 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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