

# 3«alpha»-Tigloyloxytropane

**Inchi:** InChI=1S/C13H21NO2/c1-4-9(2)13(15)16-12-7-10-5-6-11(8-12)14(10)3/h4,10-12H,5-8H2  
**InchiKey:** UVHGSMZRSVGDJ-LKQNJMEQSA-N  
**Formula:** C13H21NO2  
**SMILES:** CC=C(C)C(=O)OC1CC2CCC(C1)N2C  
**Mol. weight [g/mol]:** 223.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	2.121		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
rinpol	1646.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R411104&Units=SI>

## 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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