

# 6-Tigloyloxytropine

**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-ZRAQHMNPSA-N  
**Formula:** C13H21NO3  
**SMILES:** CC=C(C)C(=O)OC1CC2CC(O)CC1N2C  
**Mol. weight [g/mol]:** 239.31

## 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        | 1835.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R546606&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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