

# 7-tigloylretronecine

**Inchi:** InChI=1S/C13H19NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h3-4,11-12,15  
**InchiKey:** TYGYPIIOOQNWBU-ZSBMJCTGSA-N  
**Formula:** C13H19NO3  
**SMILES:** CC=C(C)C(=O)OC1CCN2CC=C(CO)C12  
**Mol. weight [g/mol]:** 237.29

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.68   |        | Crippen Method |
| logp          | 0.871   |        | Crippen Method |
| mcvol         | 187.000 | ml/mol | McGowan Method |
| rinpol        | 1815.00 |        | NIST Webbook   |
| rinpol        | 1858.00 |        | NIST Webbook   |
| rinpol        | 1815.00 |        | NIST Webbook   |
| rinpol        | 1815.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178035&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)

## 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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