

# 7-tigloyllacopsamine

**Inchi:** InChI=1S/C20H31NO6/c1-6-13(4)18(23)27-16-8-10-21-9-7-15(17(16)21)11-26-19(24)20  
**InchiKey:** MVWPTZQHBOVRTF-PQDOENCOSA-N  
**Formula:** C20H31NO6  
**SMILES:** CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)C)C(C)O)C12  
**Mol. weight [g/mol]:** 381.46

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.72   |        | Crippen Method |
| logp          | 1.190   |        | Crippen Method |
| mcvol         | 298.940 | ml/mol | McGowan Method |
| rinpola       | 2503.00 |        | NIST Webbook   |

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R516531&Units=SI>

## Legend

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

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