

# Isocallimorphine

**Inchi:** InChI=1S/C15H23NO5/c1-4-15(3,21-10(2)17)14(19)20-9-11-5-7-16-8-6-12(18)13(11)16/  
**InchiKey:** WZYYIFYCXJFFSX-QNIGDANOSA-N  
**Formula:** C15H23NO5  
**SMILES:** CCC(C)(OC(C)=O)C(=O)OCC1=CCN2CCC(O)C12  
**Mol. weight [g/mol]:** 297.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.637		Crippen Method
mcvol	226.920	ml/mol	McGowan Method
rinpol	1977.00		NIST Webbook

## Sources

**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=R178431&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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