

# Retroisosensine

**Inchi:** InChI=1S/C18H25NO5/c1-11-8-17(2)9-14(20)23-13-5-7-19-6-4-12(15(13)19)10-22-16(21)  
**InchiKey:** KOYQLXLYMDNSGL-HXEPLFAQSA-N  
**Formula:** C18H25NO5  
**SMILES:** CC1CC2(C)CC(=O)OC3CCN4CC=C(COC(=O)C1(C)O2)C34  
**Mol. weight [g/mol]:** 335.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	1.433		Crippen Method
mcvol	247.470	ml/mol	McGowan Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R636650&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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