

# Minalobine J

**Inchi:** InChI=1S/C16H27NO5/c1-4-14(18)22-11(2)16(3,20)15(19)21-10-12-7-9-17-8-5-6-13(12)  
**InchiKey:** RVTARTUVJMTYMU-LGESCRJUSA-N  
**Formula:** C16H27NO5  
**SMILES:** CCC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCCC12  
**Mol. weight [g/mol]:** 313.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	1.107		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R414356&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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