

# Minalobine R

**Inchi:** InChI=1S/C21H29NO5/c1-15(27-19(23)13-16-7-4-3-5-8-16)21(2,25)20(24)26-14-17-10-1  
**InchiKey:** FRWUADKGCTWWAT-QTQZEZTPSA-N  
**Formula:** C21H29NO5  
**SMILES:** CC(OC(=O)Cc1ccccc1)C(C)(O)C(=O)OCC1CCN2CCCC12  
**Mol. weight [g/mol]:** 375.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	1.939		Crippen Method
mcvol	292.000	ml/mol	McGowan Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R414430&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**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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