

# Minalobine K

**Inchi:** InChI=1S/C18H31NO5/c1-5-12(2)16(20)24-13(3)18(4,22)17(21)23-11-14-8-10-19-9-6-7-  
**InchiKey:** NXDDOHQAJXTHDT-BSGOTLCWSA-N  
**Formula:** C18H31NO5  
**SMILES:** CCC(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCCC12  
**Mol. weight [g/mol]:** 341.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.743		Crippen Method
mcvol	273.490	ml/mol	McGowan Method
rinpol	2142.00		NIST Webbook
rinpol	2142.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=R414361&Units=SI>

## 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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