

# 2-Methylbutyryllupinine

**Inchi:** InChI=1S/C15H27NO2/c1-3-12(2)15(17)18-11-13-7-6-10-16-9-5-4-8-14(13)16/h12-14H,3  
**InchiKey:** LFGUJSDGPHMTCB-TTZKSVMKSA-N  
**Formula:** C15H27NO2  
**SMILES:** CCC(C)C(=O)OCC1CCCN2CCCCC12  
**Mol. weight [g/mol]:** 253.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	2.840		Crippen Method
mcvol	217.910	ml/mol	McGowan Method
rinsol	1750.00		NIST Webbook
rinsol	1750.00		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=R577818&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinsol:** Non-polar retention indices

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