

# Amabiline

**Inchi:** InChI=1S/C16H27NO4/c1-10(2)16(20,11(3)18)12(4)21-9-13-5-7-17-8-6-14(19)15(13)17/  
**InchiKey:** LCGFFVMHSUIPAC-OLSVDGPUSA-N  
**Formula:** C16H27NO4  
**SMILES:** C=C(OCC1=CCN2CCC(O)C12)C(O)(C(C)C)C(C)O  
**Mol. weight [g/mol]:** 297.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	0.660		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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=R178377&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/44-201-9/Amabiline.pdf>

Generated by Cheméo on 2024-04-27 07:28:13.259544387 +0000 UTC m=+16492142.180121698.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.