

# Echimidine

**Inchi:** InChI=1S/C20H31NO7/c1-6-12(2)17(23)28-15-8-10-21-9-7-14(16(15)21)11-27-18(24)20  
**InchiKey:** HRSGCYGUWHGOPY-IMYHSKLDSA-N  
**Formula:** C20H31NO7  
**SMILES:** CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)O)C(C)(C)O)C12  
**Mol. weight [g/mol]:** 397.46  
**CAS:** 520-68-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	0.305		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
rinpola	2560.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C520683&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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>

## Legend

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

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