

# Sarracine

**Inchi:** InChI=1S/C18H27NO5/c1-4-13(3)18(22)24-15-6-8-19-7-5-14(17(15)19)11-23-16(21)9-12  
**InchiKey:** RMZXQFIAWAQDCT-NEAMIYLYSA-N  
**Formula:** C18H27NO5  
**SMILES:** CC=C(C)C(=O)OC1CCN2CCC(COC(=O)C=C(C)CO)C12  
**Mol. weight [g/mol]:** 337.41  
**CAS:** 2492-09-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.440		Crippen Method
mcvol	264.890	ml/mol	McGowan Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=C2492093&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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