

# dihydroxytriangularicine

**Inchi:** InChI=1S/C18H27NO7/c1-4-11(2)16(22)26-14-6-8-19-7-5-13(15(14)19)9-25-17(23)18(24)  
**InchiKey:** IMZYUCHNYPUYBN-GJMSPJUSA-N  
**Formula:** C18H27NO7  
**SMILES:** CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(CO)C(C)O)C12  
**Mol. weight [g/mol]:** 369.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	-0.474		Crippen Method
mcvol	276.630	ml/mol	McGowan Method
rinsol	2550.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R227979&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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