

# 7-propionylintermediate

**Inchi:** InChI=1S/C18H29NO6/c1-5-15(21)25-14-7-9-19-8-6-13(16(14)19)10-24-17(22)18(23,11)  
**InchiKey:** IZSHTSKFQLDPDL-BSXOQXRQSA-N  
**Formula:** C18H29NO6  
**SMILES:** CCC(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)C)C(C)O)C12  
**Mol. weight [g/mol]:** 355.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	0.634		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
rinpol	2300.00		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=R516526&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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