

# Timolol desisobutyl, acetylated

**Inchi:** InChI=1S/C14H21N3O5S/c1-9(18)15-7-12(22-10(2)19)8-21-14-13(16-23-17-14)11-3-5-2  
**InchiKey:** GXYLIHHCEFAPGM-GFCCVEGCSA-N  
**Formula:** C14H21N3O5S  
**SMILES:** CC(=O)NCC(COc1nsnc1C1CCOCC1)OC(C)=O  
**Mol. weight [g/mol]:** 343.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	0.879		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
rinpola	2620.00		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=R583056&Units=SI>

## 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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