

# Timolol desisobutyl - H2O, acetylated

**Inchi:** InChI=1S/C12H17N3O3S/c1-9(16)13-5-2-6-18-12-11(14-19-15-12)10-3-7-17-8-4-10/h2,5  
**InchiKey:** YQJCRGUMDPFLCP-GORDUTHDSA-N  
**Formula:** C12H17N3O3S  
**SMILES:** CC(=O)NC=CCOc1nsnc1C1CCOCC1  
**Mol. weight [g/mol]:** 283.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	1.461		Crippen Method
mcvol	204.920	ml/mol	McGowan Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		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=R583061&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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