# Timolol, acetylated

**Inchi:** InChI=1S/C18H29N3O5S/c1-12(22)21(18(3,4)5)10-15(26-13(2)23)11-25-17-16(19-27-20
**InchiKey:** PGEBILJBWXSXCG-OAHLLOKOSA-N
**Formula:** C18H29N3O5S
**SMILES:** CC(=O)OC(COc1nsnc1C1CCOCC1)CN(C(C)=O)C(C)(C)C
**Mol. weight [g/mol]:** 399.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.50 | | Crippen Method |
| logp | 2.390 | | Crippen Method |
| mcvol | 301.200 | ml/mol | McGowan Method |
| rinpol | 2290.00 | | NIST Webbook |
| rinpol | 2290.00 | | NIST Webbook |

## Sources

**Crippen Method:** 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=R583041&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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