

# Timolol

<b>Other names:</b>	2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[[4-(4-morpholinyl)-1,2,5-thiadiazol-3-yl]oxy]- (S)-1-(tert-butylamino)-3-[(4-morpholino-1,2,5-thiadiazol-3-yl)oxy]-2-propanol hemihydrate, (S)-
<b>Inchi:</b>	InChI=1S/C13H24N4O3S/c1-13(2,3)14-8-10(18)9-20-12-11(15-21-16-12)17-4-6-19-7-5-1
<b>InchiKey:</b>	BLJRIMJGRPQVNF-UHFFFAOYSA-N
<b>Formula:</b>	C13H24N4O3S
<b>SMILES:</b>	CC(C)(C)NCC(O)COc1nsnc1N1CCOCC1
<b>Mol. weight [g/mol]:</b>	316.42
<b>CAS:</b>	91524-16-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	0.503		Crippen Method
mcvol	237.590	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2262.00		NIST Webbook
rinpol	2285.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C91524162&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91524162&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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