

# Alprenolol, N-ethoxycarbonylated, TMS

**Inchi:** InChI=1S/C21H35NO4Si/c1-8-12-18-13-10-11-14-20(18)25-16-19(26-27(5,6)7)15-22(17)  
**InchiKey:** MVXAIJNKQGROAC-UHFFFAOYSA-N  
**Formula:** C<sub>21</sub>H<sub>35</sub>NO<sub>4</sub>Si  
**SMILES:** C=CCc1ccccc1OCC(CN(C(=O)OCC)C(C)C)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 393.59

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.881		Crippen Method
rinpol	2192.50		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435120&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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