

# 2-Oxacholesterol, TMS

**Inchi:** InChI=1S/C29H54O2Si/c1-20(2)10-9-11-21(3)24-14-15-25-23-13-12-22-18-27(31-32(6,7)28)16-26  
**InchiKey:** IJELOPGGEBBSQFW-PUHYIDFYSA-N  
**Formula:** C29H54O2Si  
**SMILES:** CC(C)CCCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)OCC4(C)C3CCC12C  
**Mol. weight [g/mol]:** 462.82

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	8.522		Crippen Method
rinpol	3070.00		NIST Webbook
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## 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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528737&Units=SI>

## Legend

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

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<https://www.chemeo.com/cid/37-575-3/2-Oxacholesterol-TMS.pdf>

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