

# allo-Cholanic acid, 3«alpha»,7«alpha»-dihydroxy, Me-TMS

**Other names:** 3«alpha»,7«alpha»-Dihydroxy-5«alpha»-cholanic acid, methyl ester, TMS  
**Inchi:** InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3  
**InchiKey:** FUVKOFYYHKWFJK-HFLDKKAXSA-N  
**Formula:** C31H58O4Si2  
**SMILES:** COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12O  
**Mol. weight [g/mol]:** 550.96

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
ripol	3552.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R533432&Units=SI>  
**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)

## Legend

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

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