

# Cholanic acid, 7«alpha»,12«beta»-dihydroxy, Me-TMS

**Other names:** 7«alpha»,12«beta»-Dihydroxy-5«beta»-cholanic acid, methyl ester, TMS  
**Inchi:** InChI=1S/C31H58O4Si2/c1-21(14-17-28(32)33-4)23-15-16-24-29-25(20-27(31(23,24)3)3)28-29-30-31-32-33-34-35-36-37-38-39-40-41  
**InchiKey:** WLOQXQFDQGTWNC-LFAKNFOJSA-N  
**Formula:** C31H58O4Si2  
**SMILES:** COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CCCCC4(C)C3CC(O[Si](C)(C)C)C12C  
**Mol. weight [g/mol]:** 550.96

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
ripol	3345.00		NIST Webbook
ripol	3345.00		NIST Webbook

## 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=R534297&Units=SI>

## 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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