

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

**Other names:** 7«beta»,12«alpha»-Dihydroxy-5«alpha»-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  
**InchiKey:** WLOQXQFDQGTWNC-BSKNGPBTSA-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
rinpola	3157.00		NIST Webbook
rinpola	3157.00		NIST Webbook
rinpola	3157.00		NIST Webbook
ripola	3545.00		NIST Webbook
ripola	3545.00		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=R533774&Units=SI>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/70-537-8/allo-Cholanic-acid-7-beta-12-alpha-dihydroxy-Me-TMS.pdf>

Generated by Cheméo on 2024-04-26 14:24:22.698065697 +0000 UTC m=+16430711.618643013.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.