

# allo-Cholanic acid, 3«alpha»,12«beta»-dihydroxy, Me-TMS

**Other names:** 3«alpha»,12«beta»-Dihydroxy-5«alpha»-cholanic acid, methyl ester, TMS  
**Inchi:** InChI=1S/C31H58O4Si2/c1-21(11-16-29(32)33-4)25-14-15-26-24-13-12-22-19-23(34-36)  
**InchiKey:** RDYDEBUPRPMEHW-QZDRXHTLSA-N  
**Formula:** C31H58O4Si2  
**SMILES:** COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12O  
**Mol. weight [g/mol]:** 550.96

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpola	3181.00		NIST Webbook
rinpola	3181.00		NIST Webbook
rinpola	3181.00		NIST Webbook
ripola	3552.00		NIST Webbook
ripola	3552.00		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=R533338&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

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