

# 3-«alpha»,12-«alpha»-Dihydroxy-5-«alpha»-cholanoic acid, MeTMS

Other names: 3-«alpha»-Cholanoic acid, 3-«alpha»-12-«alpha»-dihydroxy, 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)37-38-39-40  
InchiKey: RDYDEBUPRMEHW-MCQRDRPSA-N  
Formula: C31H58O4Si2  
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(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	3167.00		NIST Webbook
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rinpol	3167.00		NIST Webbook

## Sources

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=R393130&Units=SI>  
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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