

# Methyl 7-«alpha»,12«alpha»-dihydroxy-3-keto-4-cholenoate-TMS

**Other names:** 7-«alpha»,12-«alpha»-Dihydroxy-3-keto-4-cholenoic acid, MeTMS  
**Inchi:** InChI=1S/C31H54O5Si2/c1-20(11-14-28(33)34-4)23-12-13-24-29-25(19-27(31(23,24)3)32-26)/s1  
**InchiKey:** ZMFJVSCTNSUNLT-CGPUBFPPSA-N  
**Formula:** C31H54O5Si2  
**SMILES:** COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(=O)CCC4(C)C3CC(O[Si](C)(C)C)C  
**Mol. weight [g/mol]:** 562.93

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	7.384		Crippen Method
rinpol	3345.00		NIST Webbook
rinpol	3346.00		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=R393581&Units=SI>

## Legend

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

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