

# 4-Cholenoic acid, 7-«alpha»,12-«alpha»-dihydroxy, methyl ester,

**TMS**

InchiKey:

InChI=1S/C31H56O4Si2/c1-21(14-17-28(32)33-4)23-15-16-24-29-25(20-27(31(23,24)3)3

YIVNQLZONWIOQE-XXDLGFOVSA-N

Formula:

C31H56O4Si2

SMILES:

COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CCCCC4(C)C3CC(O[Si](C)(C)C)C12

Mol. weight [g/mol]:

548.94

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.205		Crippen Method
rinpol	3346.00		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=R393794&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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