

# 3-Oxo-7«alpha»,12«alpha»-dihydroxy-4-cholenic acid, methyl ester, TMS

InChI: InChI=1S/C34H62O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)33)/i1,2,3

InChIKey: SNBYLKJWRXVZKO-FKJKZISZSA-N

Formula: C<sub>34</sub>H<sub>62</sub>O<sub>5</sub>Si<sub>3</sub>

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CC(O

Mol. weight [g/mol]: 635.11

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	9.160		Crippen Method
rinpol	3360.00		NIST Webbook

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R535369&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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