

# 5-«beta»-Cholanoic acid, 3-«alpha»,4-«beta»,7-«alpha»,12-«alpha»-tetrahydroxy-methyl ester, TMS

Other names: 3-«alpha»,4-«beta»,7-«alpha»,12-«alpha»-Tetrahydroxy-5-«beta»-cholanoic acid,  
MeTMS  
Inchi: InChI=1S/C37H74O6Si4/c1-25(17-20-33(38)39-4)26-18-19-27-34-28(24-32(37(26,27)3)4

**InchiKey:** QKSYQONADMPPHH-JUVHJREISA-N

**Formula:** C37H74O6Si4

**SMILES:** COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4

**Mol. weight [g/mol]:** 727.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3455.00		NIST Webbook
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rinpol	3455.00		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=R393170&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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