# Methyl 7-«alpha»,12«alpha»-dihydroxy-3-keto-4-cholenoa 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)3
**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)
**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/ci990307l
**Crippen Method:** 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