# Methyl 5-«beta»-cholan-3,12-dione-24-oate, oxime, TMS

**Inchi:** InChI=1S/C31H56N2O4Si2/c1-21(11-16-29(34)35-4)25-14-15-26-24-13-12-22-19-23(32-

**InchiKey:** VRCDGKRYZBFSLU-BIKAVESDSA-N

**Formula:** C31H56N2O4Si2

**SMILES:** COC(=O)CCC(C)C1CCC2C3CCC4CC(=NO[Si](C)(C)C)CCC4(C)C3CC(=NO[Si](C)(C)C)

**Mol. weight [g/mol]:** 576.96

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.89 | | Crippen Method |
| logp | 8.260 | | Crippen Method |
| rinpol | 3324.00 | | NIST Webbook |
| rinpol | 3324.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R215802&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

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

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices