

# Methyl

# 5-«beta»-cholan-3-«beta»-ol-12-one-24-oate,

**oxime, TMS**  
InChI=1S/C31H57NO4Si2/c1-21(11-16-29(33)34-4)25-14-15-26-24-13-12-22-19-23(35-36)27-28  
InChIKey: BVZSXWZRUIJSAMP-QZGKGERNSA-N

**Formula:** C31H57NO4Si2

**SMILES:** COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(=NO[Si](C)(C)C)C1

**Mol. weight [g/mol]:** 563.96

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	8.272		Crippen Method
rinpol	3201.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R215966&Units=SI>

**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)

## Legend

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

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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