

# Methyl 5-«beta»-cholan-3-«alpha»,12-«alpha»-diol-7-one-oxime, TMS

InChI: InChI=1S/C34H65NO5Si3/c1-23(14-17-31(36)37-4)26-15-16-27-32-28(22-30(34(26,27)3

InChIKey: GTJMGTVXOJJKGT-IWTKPJQLSA-N

Formula: C34H65NO5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(=NO[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O

Mol. weight [g/mol]: 652.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	9.102		Crippen Method
rinpol	3276.00		NIST Webbook

## Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R215882&Units=SI>

## Legend

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

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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