

# 3-«alpha»,7-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-cholestanic acid, methyl ester, TMS

Other names:

Methyl 3-«alpha»,7-«alpha»,12-«alpha»-trihydroxy-5-«beta»cholestanoate, TMS

Inchi: InChI=1S/C37H72O5Si3/c1-25(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37)2

InchiKey: GRUORWHHLRJRJ-OSXLIQHPSA-N

Formula: C37H72O5Si3

SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC

Mol. weight [g/mol]: 681.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	10.141		Crippen Method
rinpol	3431.00		NIST Webbook
rinpol	3430.00		NIST Webbook
rinpol	3431.00		NIST Webbook

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R390037&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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