

# 3«beta»,4«beta»,12«alpha»-trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl-ether derivative

InChI: InChI=1S/C34H66O5Si3/c1-23-14-19-31(35)36(4)25-17-8-26-2-15-16-27-32(39-42(11,12)13)34  
InChIKey: HUODHVYTPQSCBY-ZCSPDBDMSA-N

SMILES: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1

Mol. weight [g/mol]: 639.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3303.00		NIST Webbook

## Sources

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)

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493166&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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