

# 3«alpha»,7«beta»,12«alpha»-Trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether

InChI: InChI=1S/C34H66O5Si3/c1-21(14-17,31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)33)/i1-3/h1-3,14-17,31,35-36,41-42,26,15-16,27-32,28(22-30(34(26,27)3)33)/t1-3,14-17,31,35-36,41-42,26,15-16,27-32,28(22-30(34(26,27)3)33)/m1

InChIKey: DQKFOBXAKZGIPX-VDIWZMOCQA-N  
Formula: C34H66O5Si3  
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(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
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=R271535&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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