Cholanoic acid, 3,6-dihydroxy, methyl ester, TMS

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-29(32)33-4)24-12-13-25-23-20-28(35-37(8,9)10)27

InchiKey: FYDBJLGZNQLQEL-DVYZTLNDSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3248.00		NIST Webbook
rinpol	3248.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394306&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices