3-«beta»,7-«alpha»-Dihydroxy-4-cholenoic acid, methyl ester, TMS

Inchi: InChI=1S/C31H56O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3

InchiKey: KHYMDYRSKURYAZ-QMTMEVIGSA-N

Formula: C31H56O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)CCC4(C)C3CCC12

Mol. weight [g/mol]: 548.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.205		Crippen Method
rinpol	3188.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390082&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices