3«beta»,7a-Dihydroxy-5-cholestenoate, MeTMS

Other names: 3-«beta»,7-«alpha»-Dihydroxy-5-cholestenoic acid, methyl ester, TMS
Inchi: InChI=1S/C34H62O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2
InchiKey: XMQRPHQEIMCXFD-NJJFLDHASA-N
Formula: C34H62O4Si2
SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 591.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	9.231		Crippen Method
rinpol	3411.00		NIST Webbook
rinpol	3415.00		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=R264423&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices