3«beta»-Hydroxy-7-oxo-5-cholestenoate, MeTMS

Inchi: InChI=1S/C34H60O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2

InchiKey: UVNOUYZSBSWLFS-DTAJUKNISA-N

Formula: C34H60O4Si2

SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3=C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3

Mol. weight [g/mol]: 589.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	9.500		Crippen Method
rinpol	3680.00		NIST Webbook
rinpol	3680.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R264443&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices