3-oxy-4,6-cholestenoate, methyl ester-trimethylsilyl ether

Inchi: InChI=1S/C31H50O3Si/c1-21(10-9-11-22(2)29(32)33-5)26-14-15-27-25-13-12-23-20-24(

InchiKey: BJLFSDGKKGSPCX-YURFGKIPSA-N

Formula: C31H50O3Si

SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C=CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C

Mol. weight [g/mol]: 498.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	8.302		Crippen Method

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=R493844&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient