3«beta»,4«beta»,7«alpha»-trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl-ether derivative

Inchi: InChI=1S/C34H66O5Si3/c1-23(11-17-30(35)36-4)24-15-16-25-31-26(18-20-33(24,25)2)3

InchiKey: XLJGJNLLTFGMTL-ZVCFGTQRSA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4(

Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3409.00		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=R493186&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices