3«alpha»,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-OLPRANPSA-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	3384.00		NIST Webbook
rinpol	3384.00		NIST Webbook
rinpol	3384.00		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=R493131&Units=SI

Legend

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