5-«alpha»-Cholanoic acid, 3-«alpha»-6-«alpha»,7-«alpha»,12-«alpha»-tetrahy methyl ester, TMS

Inchi: InChI=1S/C37H74O6Si4/c1-25(17-20-32(38)39-4)27-18-19-28-33-29(24-31(37(27,28)3)4
InchiKey: CAHBNWKLPVHQBG-HEVXDBMNSA-N
Formula: C37H74O6Si4
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(
Mol. weight [g/mol]: 727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3226.00		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=R393823&Units=SI

Legend

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