3-Oxo-7«alpha»,12«alpha»-dihydroxy-4-cholenic acid, methyl ester, TMS

Inchi: InChI=1S/C34H62O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3
InchiKey: SNBYLKJWRXVZKO-FKJKZISZSA-N
Formula: C34H62O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CC(O[
Mol. weight [g/mol]: 635.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	9.160		Crippen Method
rinpol	3360.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R535369&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