3«beta»,7«alpha»,12«alpha»-Trihydroxy-4-cholen
acid, methyl ester, TMS

Inchi: InChI=1S/C34H64O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3
InchiKey: QVMBQRVPUGQSMQ-YFJAVQHYSA-N
Formula: C34H64O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)CCC4(C)C3CC(O[S
Mol. weight [g/mol]: 637.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	9.035		Crippen Method
rinpol	3214.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R535136&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