3«alpha»,7«alpha»-dihydroxy-5«beta»-C27-bile acid, methyl ester, TMS

Inchi: InChI=1S/C34H64O4Si2/c1-23(13-12-14-24(2)32(35)36-5)27-15-16-28-31-29(18-20-34(2

InchiKey: TVTGQRYURIZRAM-QMTBGVNHSA-N

Formula: C34H64O4Si2

SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC

Mol. weight [g/mol]: 593.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	9.311		Crippen Method
rinpol	3452.00		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=R534975&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices