3-«beta»,7-«alpha»,12-«alpha»-Trihydroxy-5-chole acid, methyl ester, TMS

Inchi: InChI=1S/C37H70O5Si3/c1-25(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37(2
InchiKey: CPXIVXRFSTXASW-MSJVULRGSA-N
Formula: C37H70O5Si3
SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 679.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	10.061		Crippen Method
rinpol	3429.00		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=R390077&Units=SI

Legend

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