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

Inchi: InChI=1S/C37H72O5Si3/c1-25(16-15-17-26(2)35(38)39-5)29-18-19-30-34-31(24-33(37(2

InchiKey: GRUORWHHLRJZRJ-GYHRYELVSA-N

Formula: C37H72O5Si3

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]: 681.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	10.141		Crippen Method
rinpol	3455.00		NIST Webbook
rinpol	3455.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R534915&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