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

Other names: Methyl 3«alpha»,7«alpha»,12-«alpha»-trihydroxy-5-«beta»cholestanoate, 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-OSXLIQHPSA-N
Formula: C37H72O5Si3
SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 681.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	10.141		Crippen Method
rinpol	3431.00		NIST Webbook
rinpol	3430.00		NIST Webbook
rinpol	3431.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390037&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