3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-cholestanoic acid, MeTMS

Inchi: InChI=1S/C38H76O5Si4/c1-26(17-18-27(2)36(39)43-47(14,15)16)30-19-20-31-35-32(25-

InchiKey: KSKHCXLSDLVZLY-CIEQHBNMSA-N

Formula: C38H76O5Si4

SMILES: CC(CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C

Mol. weight [g/mol]: 725.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	10.956		Crippen Method
rinpol	3480.00		NIST Webbook
rinpol	3480.00		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=R271471&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices