5-«beta»-Cholanoic acid, 3-«alpha»,4-«beta»,7-«alpha»,12-«alpha»-tetrahyd methyl ester, TMS

Other names: 3-«alpha»,4-«beta»,7-«alpha»,12-«alpha»-Tetrahydroxy-5-«beta»-cholanoic acid, MeTMS

Inchi: InChI=1S/C37H74O6Si4/c1-25(17-20-33(38)39-4)26-18-19-27-34-28(24-32(37(26,27)3)4

InchiKey: QKSYQONADMPPHH-JUVHJREISA-N

Formula: C37H74O6Si4

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4C(O[Si](C)(C)C)C(O[Si](C)(C)C)CCC4(

Mol. weight [g/mol]: 727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3455.00		NIST Webbook
rinpol	3455.00		NIST Webbook
rinpol	3455.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393170&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices