5-Cholestenoic acid, 3-«beta»,7-«alpha»-diol, TMS

Inchi: InChI=1S/C36H68O4Si3/c1-25(15-14-16-26(2)34(37)40-43(11,12)13)29-17-18-30-33-31(

InchiKey: FPKGLSJLFHDABN-BFMVBWRGSA-N

Formula: C36H68O4Si3

SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C

Mol. weight [g/mol]: 649.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	10.436		Crippen Method
rinpol	3418.00		NIST Webbook
rinpol	3420.00		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=R177601&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices