5-Cholestenoic acid, 3-«beta»-ol-7-one, TMS

Inchi: InChI=1S/C36H66O4Si3/c1-25(15-14-16-26(2)34(37)40-43(11,12)13)29-17-18-30-33-31(
InchiKey: ZLCIYBRKMCEAQH-QUXJOQSASA-N
Formula: C36H66O4Si3
SMILES: CC(CCCC(C)C1CCC2C3=C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)
Mol. weight [g/mol]: 647.16

Physical Properties

Property code	Value	Unit	Source
logp	10.705		Crippen Method
rinpol	3775.00		NIST Webbook
rinpol	3775.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177621&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices