7«alpha»,12«alpha»-dihydroxy-3-oxy-4-chol-24-oa O-methyloxime-TMS

Inchi: InChI=1S/C34H63NO5Si3/c1-23(14-17-31(36)40-43(11,12)13)26-15-16-27-32-28(22-30(

InchiKey: GOURTNFZHFAQOS-ZECCVNMMSA-N

Formula: C34H63NO5Si3

SMILES: CON=C1C=C2CC(O[Si](C)(C)C)C3C(CC(O[Si](C)(C)C)C4(C)C(C(C)CCC(=O)O[Si](C)(C

Mol. weight [g/mol]: 650.12

Physical Properties

Property code	Value	Unit	Source
logp	9.022		Crippen Method
rinpol	3555.00		NIST Webbook
rinpol	3555.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492569&Units=SI

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

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices