Methyl 5-«beta»-cholan-7-«alpha»-12-«alpha»-diol-3-one-oxime, TMS

Inchi: InChI=1S/C34H65NO5Si3/c1-23(14-17-31(36)37-4)26-15-16-27-32-28(22-30(34(26,27)3

InchiKey: ISZZMGPQEMUNRA-NPIPRMCTSA-N

Formula: C34H65NO5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(=NO[Si](C)(C)C)CCC4(C)C3CC(O

Mol. weight [g/mol]: 652.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	9.102		Crippen Method
rinpol	3336.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R216018&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices