Methyl 5-.beta.-cholan-3,7,12-trione-24-oate, oxime, TMS # 1

Inchi: InChI=1S/C34H63N3O5Si3/c1-23(14-17-31(38)39-4)26-15-16-27-32-28(22-30(34(26,27)

InchiKey: BZYMLUPQMCEDQS-GXDNDMAQSA-N

Formula: C34H63N3O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3/C(=N/O[Si](C)(C)C)C[C@@H]4C/C(=N/O[Si](C)(C)C)CCC

Mol. weight [g/mol]: 678.15

Physical Properties

Property code	Value	Unit	Source
logp	9.077		Crippen Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R215822

Legend

logp: Octanol/Water partition coefficient