7.alpha.-hydroxy-3-oxo-4-cholestenoate, O-methyloxime, TMS (2)

Inchi: InChI=1S/C34H61NO4Si2/c1-23(13-12-14-24(2)32(36)39-41(9,10)11)27-15-16-28-31-29

InchiKey: OMMQAVPHEXZULL-NAUBTBHQSA-N

Formula: C34H61NO4Si2

SMILES: CON=C1C=C2C[C@@H](O[Si](C)(C)C)C3C(CC[C@@]4(C)C3CC[C@@H]4C(C)CCCC(

Mol. weight [g/mol]: 604.04

Physical Properties

Property code	Value	Unit	Source
logp	9.218		Crippen Method
tf	404.10	K	Cheméo Relay (1.0)

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=R492638&Units=SI

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

Legend

logp: Octanol/Water partition coefficient

tf: Normal melting (fusion) point