Methyl 5-«alpha»-cholan-3-one-24-oate, oxime, TMS # 1

Inchi: InChI=1S/C28H49NO3Si/c1-19(8-13-26(30)31-4)23-11-12-24-22-10-9-20-18-21(29-32-33

InchiKey: NPBWLYGQYCAWNA-JUCHKEMDSA-N

Formula: C28H49NO3Si

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(=NO[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 475.78

Physical Properties

Property code	Value	Unit	Source
logp	7.442		Crippen Method
rinpol	3298.00		NIST Webbook
rinpol	3298.00		NIST Webbook
tf	389.34	K	Cheméo Relay (1.0)

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?ID=R215748&Units=SI

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point