3-oxo-4-cholestenoate, O-methyloxime-TMS (1)

Inchi: InChI=1S/C31H53NO3Si/c1-21(10-9-11-22(2)29(33)35-36(6,7)8)26-14-15-27-25-13-12-2

InchiKey: HOMDZWFYFIHOMY-YURFGKIPSA-N

Formula: C31H53NO3Si

SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)CCCC(C)C(=O)O[Si](C)(C)C)CCC34)C2(C)CC1

Mol. weight [g/mol]: 515.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	8.388		Crippen Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492529&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices