Methyl 5-«beta»-cholan-7-«alpha»-ol-3-one-24-oate, oxime, TMS #2

Inchi: InChI=1S/C31H57NO4Si2/c1-21(11-14-28(33)34-4)24-12-13-25-29-26(16-18-31(24,25)3

InchiKey: CQTMZNGJGAEHPX-JRWHHOMKSA-N

Formula: C31H57NO4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(=NO[Si](C)(C)C)CCC4(C)C3CCC1

Mol. weight [g/mol]: 563.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.35		Cheméo Relay (1.0)
logp	8.272		Crippen Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R216043&Units=SI

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):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices