Methyl 5-.beta.-cholan-7-.alpha.-ol-3-one-24-oate, oxime, TMS #1

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-KZUUWTDGSA-N
Formula: C31H57NO4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3C(CCC12C)C1(C)CC/C(=N/O[Si](C)(C)C)C[C@H]1C[C@H
Mol. weight [g/mol]: 563.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Cheméo Relay (1.0)
logp	8.272		Crippen Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R216038
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):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient