Methyl 5-.beta.-cholan-12-.alpha.-ol-3-one-24-oate, oxime, TMS #2

Inchi: InChI=1S/C31H57NO4Si2/c1-21(11-16-29(33)34-4)25-14-15-26-24-13-12-22-19-23(32-3

InchiKey: QIWSBVFPWMELCB-BNVKNMGISA-N

Formula: C31H57NO4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3CC[C@@H]4C/C(=N/O[Si](C)(C)C)CCC4(C)C3C[C@H](O[

Mol. weight [g/mol]: 563.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Cheméo Relay (1.0)
logp	8.272		Crippen Method

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?Str2File=R215788

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