Methyl 5-«beta»-cholan-3-«beta»-ol-12-one-24-oate, oxime, TMS

Inchi: InChI=1S/C31H57NO4Si2/c1-21(11-16-29(33)34-4)25-14-15-26-24-13-12-22-19-23(35-3

InchiKey: BVZSXWZRUJSAMP-QZGKGERNSA-N

Formula: C31H57NO4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(=NO[Si](C)(C)C)C1

Mol. weight [g/mol]: 563.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	8.272		Crippen Method
rinpol	3201.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R215966&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices