Methyl chol-4-en-3,7,12-trione-24-oate, oxime, TMS

Inchi: InChI=1S/C34H61N3O5Si3/c1-23(14-17-31(38)39-4)26-15-16-27-32-28(22-30(34(26,27)

InchiKey: YOGKVDANCQTORX-UHFFFAOYSA-N

Formula: C34H61N3O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(=NO[Si](C)(C)C)CC4=CC(=NO[Si](C)(C)C)CCC4(C)C3C

Mol. weight [g/mol]: 676.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	8.997		Crippen Method
rinpol	3538.00		NIST Webbook
rinpol	3538.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R216083&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