7«alpha»-hydroxy-3-oxo-4-chol-24-oate, O-methyloxime, TMS (1)

Inchi: InChI=1S/C31H55NO4Si2/c1-21(11-14-28(33)36-38(8,9)10)24-12-13-25-29-26(16-18-31

InchiKey: QOTVZIAXEYHVPF-PEXYKONISA-N

Formula: C31H55NO4Si2

SMILES: CON=C1C=C2CC(O[Si](C)(C)C)C3C(CCC4(C)C(C(C)CCC(=O)O[Si](C)(C)C)CCC34)C2

Mol. weight [g/mol]: 561.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	8.192		Crippen Method
rinpol	3250.00		NIST Webbook
rinpol	3265.00		NIST Webbook
rinpol	3250.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492252&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