7«alpha»-hydroxy-3-oxo-4-chol-24-oate, oxime-TMS

Inchi: InChI=1S/C33H61NO4Si3/c1-23(13-16-30(35)37-40(7,8)9)26-14-15-27-31-28(18-20-33(2

InchiKey: WSIKZUQMLAIGEC-RILFYBJCSA-N

Formula: C33H61NO4Si3

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

Mol. weight [g/mol]: 620.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	9.397		Crippen Method
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492589&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