4-Cholestenoic acid, 3-one, TMS

Inchi: InChI=1S/C33H58O3Si2/c1-23(12-11-13-24(2)31(34)36-38(8,9)10)28-16-17-29-27-15-14
InchiKey: AEVYTVYTETXXGC-VDNSYZNFSA-N
Formula: C33H58O3Si2
SMILES: CC(CCCC(C)C1CCC2C3CCC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C)C(=O)O[Si](C)(
Mol. weight [g/mol]: 558.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	9.731		Crippen Method
rinpol	3528.00		NIST Webbook
rinpol	3528.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177458&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