4-Cholenoic acid, 3-one, TMS

Inchi: InChI=1S/C30H52O3Si2/c1-21(10-15-28(31)33-35(7,8)9)25-13-14-26-24-12-11-22-20-23
InchiKey: ABLNXOFFQVZHLO-DICFPEKDSA-N
Formula: C30H52O3Si2
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3CCC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C
Mol. weight [g/mol]: 516.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	8.705		Crippen Method
rinpol	3265.00		NIST Webbook
rinpol	3265.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177369&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices