7«alpha»,25-Dihydroxy-4-cholesten-3-one, TMS

Inchi: InChI=1S/C36H68O3Si3/c1-26(16-15-21-34(2,3)39-42(12,13)14)29-17-18-30-33-31(20-2

InchiKey: DDTVWJWLYFOTPG-YILISMQQSA-N

Formula: C36H68O3Si3

SMILES: CC(CCCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4C=C(O[Si](C)(C)C)CCC4

Mol. weight [g/mol]: 633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	11.177		Crippen Method
rinpol	3490.00		NIST Webbook
rinpol	3490.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R264458&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