5-Cholenoic acid, 3-«beta»,7-«beta»-diol, TMS

Inchi: InChI=1S/C36H70O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36
InchiKey: ACPUMZZEKMSBSV-ZKVVBUKYSA-N
Formula: C36H70O5Si4
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C
Mol. weight [g/mol]: 695.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	10.240		Crippen Method
rinpol	3302.00		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=R177498&Units=SI

Legend

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