5-Cholenoic acid, 3-«beta»,7-«alpha»-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-JTQVGFLKSA-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	3185.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177483&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