5-Cholesten-3-«beta»,7-«alpha»,12-«alpha»,25-tet
TMS

InChI: InChI=1S/C39H78O4Si4/c1-28(19-18-23-37(2,3)43-47(15,16)17)31-20-21-32-36-33(27-3

InchiKey: PKNLLDOYGGFAIH-FGWGIACJSA-N

Formula: C39H78O4Si4

SMILES: CC(CCCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(

Mol. weight [g/mol]: 723.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	11.882		Crippen Method
rinpol	3396.00		NIST Webbook
rinpol	3396.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390200&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