5-Cholesten-3-«beta»,27-diol-17,22-dione, TMS

Inchi: InChI=1S/C39H74O4Si4/c1-28(17-20-35(42-46(11,12)13)29(2)27-40-44(5,6)7)32-18-19-3
InchiKey: FVZLXJKNOFHPED-RCWLVPAYSA-N
Formula: C39H74O4Si4
SMILES: CC(CO[Si](C)(C)C)=C(CCC(C)C1CCC2C3=C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC
Mol. weight [g/mol]: 719.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	12.278		Crippen Method
rinpol	3795.00		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=R177532&Units=SI

Legend

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