3,11,20,21-Tetrahydroxypregnane, tetrakis-TMS

Inchi: InChI=1S/C33H68O4Si4/c1-32-20-19-25(35-39(6,7)8)21-24(32)15-16-26-27-17-18-28(30

InchiKey: RUHLXDLUNAJPIW-UHFFFAOYSA-N

Formula: C33H68O4Si4

SMILES: CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2C(CO[Si](C)(C)C)

Mol. weight [g/mol]: 641.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.41		Crippen Method
logp	9.767		Crippen Method
rinpol	3158.00		NIST Webbook
rinpol	3158.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R16545&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