Thromboxane B2, reduced, tetrakis-TMS

Inchi: InChI=1S/C32H68O6Si4/c1-14-15-18-21-28(36-40(5,6)7)24-25-30(33)29(22-19-16-17-20
InchiKey: VTFFYSQOZOUVSJ-TZXMBOKHSA-N
Formula: C32H68O6Si4
SMILES: CCCCCC(C=CC(O)C(CC=CCCCC(=O)O[Si](C)(C)C)C(CCO[Si](C)(C)C)O[Si](C)(C)C)O[
Mol. weight [g/mol]: 661.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.61		Crippen Method
logp	9.277		Crippen Method
rinpol	2820.00		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=R526568&Units=SI

Legend

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