15-Keto-PGE2, BO-TMS, isomer # 1

Inchi: InChI=1S/C34H64N2O5Si2/c1-10-13-18-21-29(35-38-26-14-11-2)24-25-31-30(22-19-16-
InchiKey: RMJAGIVEDWGGNH-WVFVVGEFSA-N
Formula: C34H64N2O5Si2
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NO
Mol. weight [g/mol]: 637.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.82		Crippen Method
logp	9.819		Crippen Method
rinpol	3048.00		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=R581134&Units=SI

Legend

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