13,14-Dihydro-15-keto-PGE2, BO-TMS, isomer # 4

Inchi: InChI=1S/C34H66N2O5Si2/c1-10-13-18-21-29(35-38-26-14-11-2)24-25-31-30(22-19-16-

InchiKey: GVSHYYIQRKPSGU-ORGQUXCYSA-N

Formula: C34H66N2O5Si2

SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NOC

Mol. weight [g/mol]: 639.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	10.043		Crippen Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580557&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