13,14-Dihydro-6,15-diketo-PGF1A, BO-TMS, isomer # 1

Inchi: InChI=1S/C37H76N2O6Si3/c1-13-16-19-22-31(38-41-27-17-14-2)25-26-33-34(36(44-47(

InchiKey: LQTFTWUJGAVZNV-SKXFTCKDSA-N

Formula: C37H76N2O6Si3

SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC(CCCCC(=O)O[Si](C)(C)C)=NO

Mol. weight [g/mol]: 729.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	11.097		Crippen Method
rinpol	3155.00		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=R580824&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices