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

Inchi: InChI=1S/C31H64N2O6Si3/c1-13-14-15-18-25(32-35-2)21-22-27-28(30(38-41(7,8)9)24-2

InchiKey: VIPQHXNLXJXFOZ-GCXHJFECSA-N

Formula: C31H64N2O6Si3

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]: 645.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	8.757		Crippen Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580899&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices