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

Inchi: InChI=1S/C33H68N2O6Si3/c1-13-16-17-20-27(34-37-14-2)23-24-29-30(32(40-43(7,8)9)2

InchiKey: NFECWVKGLYDHML-RTNMLALUSA-N

Formula: C33H68N2O6Si3

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]: 673.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	9.537		Crippen Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		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=R580864&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices