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

Inchi: InChI=1S/C28H52N2O5Si2/c1-10-11-14-17-23(29-32-2)20-21-25-24(26(30-33-3)22-27(2
InchiKey: LWEGMMOMOPWUPC-MDOVGBOESA-N
Formula: C28H52N2O5Si2
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NOC
Mol. weight [g/mol]: 552.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	7.479		Crippen Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		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=R581218&Units=SI

Legend

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