15-Keto-PGA2A, EO-TMS, isomer # 1

Inchi: InChI=1S/C27H46N2O4Si/c1-7-10-13-16-24(28-31-8-2)21-19-23-20-22-26(29-32-9-3)25(
InchiKey: MPRFRKVLHCOXCQ-FQMMLSTLSA-N
Formula: C27H46N2O4Si
SMILES: CCCCCC(C=CC1C=CC(=NOCC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NOCC
Mol. weight [g/mol]: 490.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	7.205		Crippen Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		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=R581109&Units=SI

Legend

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