15-Keto-PGA1A, EO-TMS, isomer # 2

Inchi: InChI=1S/C27H48N2O4Si/c1-7-10-13-16-24(28-31-8-2)21-19-23-20-22-26(29-32-9-3)25(
InchiKey: RJRAIJIKIHSVOZ-RARVZMPBSA-N
Formula: C27H48N2O4Si
SMILES: CCCCCC(C=CC1C=CC(=NOCC)C1CCCCCCC(=O)O[Si](C)(C)C)=NOCC
Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
logp	7.429		Crippen Method
rinpol	2795.00		NIST Webbook
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
rinpol	2795.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581050&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices