15-Keto-PGE2, EO-TMS, isomer # 4

Inchi: InChI=1S/C30H56N2O5Si2/c1-10-13-16-19-25(31-34-11-2)22-23-27-26(20-17-14-15-18-
InchiKey: SYKNYLRBRFILLL-QPZUBDORSA-N
Formula: C30H56N2O5Si2
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCC)C1CC=CCCCC(=O)O[Si](C)(C)C)=NOCC
Mol. weight [g/mol]: 580.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	8.259		Crippen Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		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=R581203&Units=SI

Legend

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

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