13,14-Dihydro-PGE2, BO-TMS, isomer # 1

Inchi: InChI=1S/C33H67NO5Si3/c1-12-14-18-21-28(37-40(3,4)5)24-25-30-29(22-19-16-17-20-2
InchiKey: QTNUVEXAKJMSSK-ZUSCEGDDSA-N
Formula: C33H67NO5Si3
SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C
Mol. weight [g/mol]: 642.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	10.091		Crippen Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R580973&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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