PGD1, EO-TMS, isomer # 1

Inchi: InChI=1S/C31H63NO5Si3/c1-12-14-17-20-26(35-38(3,4)5)23-24-27-28(21-18-15-16-19-2
InchiKey: KZUHVQWLOMUWAS-BPXHILEUSA-N
Formula: C31H63NO5Si3
SMILES: CCCCCC(C=CC1C(=NOCC)CC(O[Si](C)(C)C)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C
Mol. weight [g/mol]: 614.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	9.310		Crippen Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		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=R581738&Units=SI

Legend

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