PGD2, BO-TMS, isomer # 1

Inchi: InChI=1S/C33H65NO5Si3/c1-12-14-18-21-28(37-40(3,4)5)24-25-29-30(22-19-16-17-20-2
InchiKey: BGDMMRPKSLKJCY-GKYVNCFCSA-N
Formula: C33H65NO5Si3
SMILES: CCCCCC(C=CC1C(=NOCCCC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si]
Mol. weight [g/mol]: 640.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	9.867		Crippen Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		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=R581778&Units=SI

Legend

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