15(S)-15-Methyl-PGA2, BO-TMS, isomer # 2

Inchi: InChI=1S/C31H57NO4Si2/c1-10-12-18-24-31(3,36-38(7,8)9)25-23-27-21-22-29(32-34-26
InchiKey: PFHNSQOPBICNCF-CWZPGBDYSA-N
Formula: C31H57NO4Si2
SMILES: CCCCCC(C)(C=CC1C=CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 563.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	9.203		Crippen Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581278&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