15(S)-15-Methyl-PGD2, EO-TMS, isomer # 1

Inchi: InChI=1S/C32H63NO5Si3/c1-13-15-20-24-32(3,38-41(10,11)12)25-23-27-28(21-18-16-1
InchiKey: ZVCQJBNGECDLRP-MVTDFAKDSA-N
Formula: C32H63NO5Si3
SMILES: CCCCCC(C)(C=CC1C(=NOCC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si]
Mol. weight [g/mol]: 626.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	9.476		Crippen Method
rinpol	2741.00		NIST Webbook
rinpol	2741.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581367&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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