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

Inchi: InChI=1S/C31H61NO5Si3/c1-13-14-19-23-31(2,37-40(10,11)12)24-22-26-27(29(35-38(4
InchiKey: FVRPOQAWAKAVRZ-IYPQQAMXSA-N
Formula: C31H61NO5Si3
SMILES: CCCCCC(C)(C=CC1C(=NOC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C
Mol. weight [g/mol]: 612.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	9.086		Crippen Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R581387&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

Latest version available from:
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