15(S)-15-Methyl-PGD2, BO-TMS

Inchi: InChI=1S/C34H67NO5Si3/c1-13-15-21-25-34(3,40-43(10,11)12)26-24-29-30(22-19-17-1
InchiKey: GJZRQHSQVCXDPJ-GHQZTLPXSA-N
Formula: C34H67NO5Si3
SMILES: CCCCCC(C)(C=CC1C(=NOCCCC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O
Mol. weight [g/mol]: 654.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	10.257		Crippen Method
rinpol	2913.00		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=R581352&Units=SI

Legend

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