Prostaglandin D(2), O,O'-bis(trimethylsilyl)-, trimethylsilyl ester

Inchi: InChI=1S/C29H56O5Si3/c1-11-12-15-18-24(32-35(2,3)4)21-22-25-26(28(23-27(25)30)33

InchiKey: XATDHEXRHMXFAW-LBWJEKIOSA-N

Formula: C29H56O5Si3

SMILES: CCCCCC(C=CC1C(=O)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 569.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	8.263		Crippen Method
rinpol	2795.70		NIST Webbook
rinpol	2795.70		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U334029&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