PGD2 TMS

Inchi: InChI=1S/C29H58O4Si3/c1-11-12-15-18-26(31-34(2,3)4)23-21-25-22-24-28(32-35(5,6)7)
InchiKey: RZLAFOZHYPFJLC-YJFZFQCTSA-N
Formula: C29H58O4Si3
SMILES: CCCCCC(C=CC1CCC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 555.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	9.084		Crippen Method
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R16862&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