11«alpha»,15«alpha»-dihydroxy-9-ketoprosta-5,13 acid, MO TMS #1

Inchi: InChI=1S/C31H61NO5Si3/c1-13-14-19-23-31(2,37-40(10,11)12)24-22-27-26(28(32-34-3)
InchiKey: XQFHPVCJGCPJIN-QHVDWANMSA-N
Formula: C31H61NO5Si3
SMILES: CCCCCC(C)(C=CC1C(O[Si](C)(C)C)CC(=NOC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C
Mol. weight [g/mol]: 612.08

Physical Properties

Property code	Value	Unit	Source
logp	9.086		Crippen Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R385609&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices