

13,14-Dihydro-PGE2, BO-TMS, isomer # 1

Inchi: InChI=1S/C33H67NO5Si3/c1-12-14-18-21-28(37-40(3,4)5)24-25-30-29(22-19-16-17-20-23)O/Si(C)(C)C/Si(C)(C)C
InchiKey: QTNUVEXAKJMSSK-ZUSCEGDDSA-N
Formula: C33H67NO5Si3
SMILES: CCCCC(CCC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 642.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	10.091		Crippen Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580973&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/122-911-4/13-14-Dihydro-PGE2-BO-TMS-isomer-1.pdf>

Generated by Cheméo on 2024-05-03 18:27:25.259467742 +0000 UTC m=+17050094.180045057.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.