PGE1, EO-TMS, isomer # 1

Inchi:	InChI=1S/C31H63NO5Si3/c1-12-14-17-20-26(35-38(3,4)5)23-24-28-27(21-18-15-16-19-2
InchiKey:	OPGNTQXLISFYMW-PIWXXMLHSA-N
Formula:	C31H63NO5Si3
SMILES:	CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(
Mol. weight [g/mol]:	614.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	9.310		Crippen Method
rinpol	2751.00		NIST Webbook
rinpol	2751.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R581852&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

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