

PGE1, 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)O/Si(C)(C)C(Si(C)(C)C)O
InchiKey: OJXHJQKCVJNAAN-ZXUAAGSQSA-N
Formula: C33H67NO5Si3
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C(Si(C)(C)C)O
Mol. weight [g/mol]: 642.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	10.091		Crippen Method
rinpol	2904.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581832&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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.chemeo.com/cid/114-015-8/PGE1-BO-TMS-isomer-1.pdf>

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