

PGE2, BO-TMS, isomer # 2

Inchi: InChI=1S/C33H65NO5Si3/c1-12-14-18-21-28(37-40(3,4)5)24-25-30-29(22-19-16-17-20-23)31-32-33
InchiKey: KNYXDDWQYFOOER-BTZWMAIRSA-N
Formula: C33H65NO5Si3
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(=NOCCCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 640.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	9.867		Crippen Method
rinpol	2954.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581901&Units=SI>

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/70-959-0/PGE2-BO-TMS-isomer-2.pdf>

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