

PGD2, EO-TMS, isomer # 1

Inchi: InChI=1S/C31H61NO5Si3/c1-12-14-17-20-26(35-38(3,4)5)23-24-27-28(21-18-15-16-19-20)
InchiKey: PDWLFNBOHCWZAX-ZKXNLKAOSA-N
Formula: C31H61NO5Si3
SMILES: CCCCCC(C=CC1C(=NOCC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 612.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	9.086		Crippen Method
rinsol	2731.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581798&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/117-231-5/PGD2-EO-TMS-isomer-1.pdf>

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