

PGD2, MO-TMS, isomer # 1

Inchi: InChI=1S/C30H59NO5Si3/c1-12-13-16-19-25(34-37(3,4)5)22-23-26-27(29(35-38(6,7)8)2
InchiKey: JMMSMDXQYZWEDQ-KGNSKYJBSA-N
Formula: C30H59NO5Si3
SMILES: CCCCCC(C=CC1C(=NOC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 598.05

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.15 | | Crippen Method |
| logp | 8.696 | | Crippen Method |
| rinpol | 2676.00 | | NIST Webbook |
| rinpol | 2676.00 | | NIST Webbook |

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=R581812&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/113-560-4/PGD2-MO-TMS-isomer-1.pdf>

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