

13,14-Dihydro-15-keto-PGE2, EO-TMS, isomer # 2

Inchi: InChI=1S/C30H58N2O5Si2/c1-10-13-16-19-25(31-34-11-2)22-23-27-26(20-17-14-15-18-19)/n1-2
InchiKey: UWXDFULQJFGIIN-OPNXPFFOSA-N
Formula: C30H58N2O5Si2
SMILES: CCCCCC(CCC1C(O[Si](C)(C)C)CC(=NOCC)C1CC=CCCC(=O)O[Si](C)(C)C)=NOCC
Mol. weight [g/mol]: 582.96

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.29 | | Crippen Method |
| logp | 8.483 | | Crippen Method |
| rinpol | 2803.00 | | NIST Webbook |
| rinpol | 2803.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580577&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/69-858-4/13-14-Dihydro-15-keto-PGE2-EO-TMS-isomer-2.pdf>

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