

15-Keto-PGA1A, BO-TMS, isomer # 2

Inchi: InChI=1S/C31H56N2O4Si/c1-7-10-15-18-28(32-35-25-11-8-2)23-21-27-22-24-30(33-36-2)
InchiKey: LSOMCPVJIKZVAL-VPSOQQPASA-N
Formula: C31H56N2O4Si
SMILES: CCCCCC(C=CC1C=CC(=NOCCCC)C1CCCCCCC(=O)O[Si](C)(C)C)=NOCCCC
Mol. weight [g/mol]: 548.87

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -7.31 | | Crippen Method |
| logp | 8.989 | | Crippen Method |
| rinpol | 2956.00 | | NIST Webbook |
| rinpol | 2956.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581045&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/121-353-5/15-Keto-PGA1A-BO-TMS-isomer-2.pdf>

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