

15-Keto-PGA1A, MO-TMS

Inchi: InChI=1S/C25H44N2O4Si/c1-7-8-11-14-22(26-29-2)19-17-21-18-20-24(27-30-3)23(21)15
InchiKey: SZJSHSSEGPVEOP-UUTDRFNZSA-N
Formula: C25H44N2O4Si
SMILES: CCCCCC(C=CC1C=CC(=NOC)C1CCCCCCC(=O)O[Si](C)(C)C)=NOC
Mol. weight [g/mol]: 464.71

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.80 | | Crippen Method |
| logp | 6.649 | | Crippen Method |
| rinpol | 2744.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581070&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.cheméo.com/cid/60-655-8/15-Keto-PGA1A-MO-TMS.pdf>

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