

PGA2, EO-TMS, isomer # 2

Inchi: InChI=1S/C28H51NO4Si2/c1-9-11-14-17-25(32-34(3,4)5)22-20-24-21-23-27(29-31-10-2)
InchiKey: FAIKGANMUMFBOQ-TYRFPOHKSA-N
Formula: C28H51NO4Si2
SMILES: CCCCCC(C=CC1C=CC(=NOCC)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 521.88

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.92 | | Crippen Method |
| logp | 8.032 | | Crippen Method |
| rinpol | 2631.00 | | NIST Webbook |
| rinpol | 2631.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581629&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/113-120-2/PGA2-EO-TMS-isomer-2.pdf>

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