

19-Hydroxy PGA1 TMS

Inchi: InChI=1S/C29H56O5Si3/c1-24(32-35(2,3)4)16-15-17-26(33-36(5,6)7)22-20-25-21-23-28
InchiKey: HCMBMNGIEWXBJR-JKLMWWWKPSA-N
Formula: C29H56O5Si3
SMILES: CC(CCCC(C=CC1C=CC(=O)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 569.01

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.77 | | Crippen Method |
| logp | 8.263 | | Crippen Method |
| rinpol | 3241.00 | | 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=R16773&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/22-515-5/19-Hydroxy-PGA1-TMS.pdf>

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