

12-«alpha»-Hydroxy-GA5, MeTMSi

Inchi: InChI=1S/C26H40O6Si2/c1-16-14-24-15-26(16,32-34(7,8)9)18(31-33(4,5)6)13-17(24)25-26
InchiKey: KQGUPRWOMUWGHL-WFMOHTBYSA-N
Formula: C26H40O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)O1
Mol. weight [g/mol]: 504.76

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.02 | | Crippen Method |
| logp | 4.834 | | Crippen Method |
| rinpol | 2641.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79042&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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/48-677-8/12-alpha-Hydroxy-GA5-MeTMSi.pdf>

Generated by Cheméo on 2024-04-19 00:30:42.892253287 +0000 UTC m=+15775891.812830599.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.