

Pregnanediol MO TMS

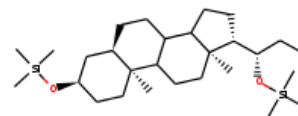
InChI: InChI=1S/C28H54O2Si2/c1-10-26(30-32(7,8)9)25-14-13-23-22-12-11-20-19-21(29-31(4,5)6)15-17-27(20,2)24(22)16-18-28(23,25)3/h20-26H,10-19H2,1-9H3/t20-,21-,22?,23?,24?,25-,26+,27+,28+/m0/s1

InChI Key: FFOITQMJIMFGSD-SAGLKEOOSA-N

Formula: C28H54O2Si2

SMILES: CCC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Molecular Weight: 478.90



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 8.496 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H54O2Si2/c1-10-26\(30-32\(7,8\)9\)25-14-13-23-22-12-11-20-19-21\(29-31\(4,5\)6\)15-17-27\(20,2\)24\(22\)16-18-28\(23,25\)3/h20-26H,10-19H2,1-9H3/t20-,21-,22?,23?,24?,25-,26+,27+,28+/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H54O2Si2/c1-10-26(30-32(7,8)9)25-14-13-23-22-12-11-20-19-21(29-31(4,5)6)15-17-27(20,2)24(22)16-18-28(23,25)3/h20-26H,10-19H2,1-9H3/t20-,21-,22?,23?,24?,25-,26+,27+,28+/m0/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

Latest version available from:

<https://old.cheméo.com/cid/19-887-7/Pregnanediol%20MO%20TMS>

Generated by Cheméo on Mon, 08 Aug 2022 23:26:33 +0000.

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