

5-«alpha»-Pregnan-3,17,20-triol, MeTMS

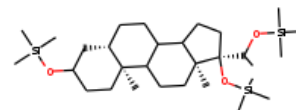
InChI: InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21-24(32-35(7,8)9)15-18-28(23,2)26(25)16-19-29(27,30)3/h22-27H,13-21H2,1-12H3/t22?,23-,24?,25?,26?,27?,28-,29-,30?/m1/s1

InChI Key: KFUWLVZCEDFJIK-OOURMZHRSA-N

Formula: C30H60O3Si3

SMILES: CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Molecular Weight: 553.05



Physical Properties

| Property | Value | Unit | Source |
|---------------------------|-------|------|----------------|
| $\log P_{\text{oct/wat}}$ | 9.08 | | Crippen Method |

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C30H60O3Si3/c1-22\(31-34\(4,5\)6\)30\(33-36\(10,11\)12\)20-17-27-25-14-13-23-21-24\(32-35\(7,8\)9\)15-18-28\(23,2\)26\(25\)16-19-29\(27,30\)3/h22-27H,13-21H2,1-12H3/t22?,23-,24?,25?,26?,27?,28-,29-,30?/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21-24(32-35(7,8)9)15-18-28(23,2)26(25)16-19-29(27,30)3/h22-27H,13-21H2,1-12H3/t22?,23-,24?,25?,26?,27?,28-,29-,30?/m1/s1)

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

Legend

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

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