

5-«beta»-Pregnan-3-«beta»,20-«alpha»-diol, TMS

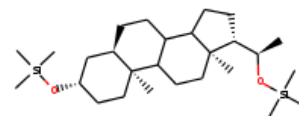
InChI: InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)14-16-26(20,2)25(22)15-17-27(23,24)3/h19-25H,10-18H2,1-9H3/t19-,20-,21+,22?,23-,24?,25?,26+,27-/m0/s1

InChI Key: PSZRAFDARWUCMW-JOPQZIHYSAN

Formula: C₂₇H₅₂O₂Si₂

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

Molecular Weight: 464.87



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	8.105		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H52O2Si2/c1-19\(28-30\(4,5\)6\)23-12-13-24-22-11-10-20-18-21\(29-31\(7,8\)9\)14-16-26\(20,2\)25\(22\)15-17-27\(23,24\)3/h19-25H,10-18H2,1-9H3/t19-,20-,21+,22?,23-,24?,25?,26+,27-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)14-16-26(20,2)25(22)15-17-27(23,24)3/h19-25H,10-18H2,1-9H3/t19-,20-,21+,22?,23-,24?,25?,26+,27-/m0/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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