

5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha»-triol, (3,20-O)-diTBDMSi

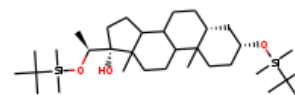
InChI: InChI=1S/C33H64O3Si2/c1-23(35-37(10,11)29(2,3)4)33(34)21-18-28-26-15-14-24-22-25(36-38(12,13)30(5,6)7)16-19-31(24,8)27(26)17-20-32(28,33)9/h23-28,34H,14-22H2,1-13H3/t23-,24+,25+,26?,27?,28?,31?,32?,33-/m1/s1

InChI Key: GHNXJGWJFKLUHM-ZNWXLFBDNA-N

Formula: C₃₃H₆₄O₃Si₂

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

Molecular Weight: 565.03



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	9.56		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C33H64O3Si2/c1-23\(35-37\(10,11\)29\(2,3\)4\)33\(34\)21-18-28-26-15-14-24-22-25\(36-38\(12,13\)30\(5,6\)7\)16-19-31\(24,8\)27\(26\)17-20-32\(28,33\)9/h23-28,34H,14-22H2,1-13H3/t23-,24+,25+,26?,27?,28?,31?,32?,33-/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C33H64O3Si2/c1-23(35-37(10,11)29(2,3)4)33(34)21-18-28-26-15-14-24-22-25(36-38(12,13)30(5,6)7)16-19-31(24,8)27(26)17-20-32(28,33)9/h23-28,34H,14-22H2,1-13H3/t23-,24+,25+,26?,27?,28?,31?,32?,33-/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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