

1-Methyl-6.alpha.,7.alpha.-dihydroxyestrone, TMS

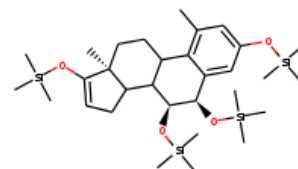
InChI: InChI=1S/C31H56O4Si4/c1-21-19-22(32-36(3,4)5)20-24-27(21)23-17-18-31(2)25(15-16-26(31)33-37(6,7)8)28(23)30(35-39(12,13)14)29(24)34-38(9,10)11/h16,19-20,23,25,28-30H,15,17-18H2,1-14H3/t23?,25?,28?,29-,30+,31+/m0/s1

InChI Key: ANTMMWDLXLMSNB-OYWOUPIPSA-N

Formula: C₃₁H₅₆O₄Si₄

SMILES: Cc1cc(O[Si](C)(C)C)cc2c1C1CCC3(C)C(O[Si](C)(C)C)=CCC3C1C(O[Si](C)(C)C)C2O[Si](C)(C)C

Molecular Weight: 605.12



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	9.59		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C31H56O4Si4/c1-21-19-22\(32-36\(3,4\)5\)20-24-27\(21\)23-17-18-31\(2\)25\(15-16-26\(31\)33-37\(6,7\)8\)28\(23\)30\(35-39\(12,13\)14\)29\(24\)34-38\(9,10\)11/h16,19-20,23,25,28-30H,15,17-18H2,1-14H3/t23?,25?,28?,29-,30+,31+/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C31H56O4Si4/c1-21-19-22(32-36(3,4)5)20-24-27(21)23-17-18-31(2)25(15-16-26(31)33-37(6,7)8)28(23)30(35-39(12,13)14)29(24)34-38(9,10)11/h16,19-20,23,25,28-30H,15,17-18H2,1-14H3/t23?,25?,28?,29-,30+,31+/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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