

7«alpha»,26-dihydroxy-4-cholesten-3-one, TMS

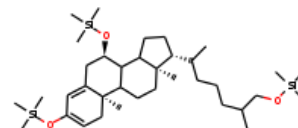
InChI: InChI=1S/C36H68O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)30-17-18-31-34-32(20-22-36(30,31)4)35(3)21-19-29(38-41(8,9)10)23-28(35)24-33(34)39-42(11,12)13/h19,23,26-27,30-34H,14-18,20-22,24-25H2,1-13H3/t26?,27?,30-,31?,32?,33-,34?,35+,36-/m0/s1

InChI Key: LVBALRWAXSVALG-BLLMLTCESA-N

Formula: C₃₆H₆₈O₃Si₃

SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C)CO[Si](C)(C)C

Molecular Weight: 633.18



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	11.035		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C36H68O3Si3/c1-26\(25-37-40\(5,6\)7\)15-14-16-27\(2\)30-17-18-31-34-32\(20-22-36\(30,31\)4\)35\(3\)21-19-29\(38-41\(8,9\)10\)23-28\(35\)24-33\(34\)39-42\(11,12\)13/h19,23,26-27,30-34H,14-18,20-22,24-25H2,1-13H3/t26?,27?,30-,31?,32?,33-,34?,35+,36-/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C36H68O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)30-17-18-31-34-32(20-22-36(30,31)4)35(3)21-19-29(38-41(8,9)10)23-28(35)24-33(34)39-42(11,12)13/h19,23,26-27,30-34H,14-18,20-22,24-25H2,1-13H3/t26?,27?,30-,31?,32?,33-,34?,35+,36-/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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