

# 5«alpha»-Cholestan-3«alpha»,6«beta»-diol, VDMS

**Inchi:** InChI=1S/C35H64O2Si2/c1-12-38(8,9)36-27-19-21-35(7)31-20-22-34(6)29(26(5)16-14-13)28-32-33-37-30-23-24-25-26-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/h1-34,38-41,43-45,47-49,51-53,55-57,59-61,63-65,67-69,71-73,75-77,79-81,83-85,87-89,91-93,95-97,99-100/t1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31,33,35,37,39,41,43,45,47,49,51,53,55,57,59,61,63,65,67,69,71,73,75,77,79,81,83,85,87,89,91,93,95,97,99-100/m-1/s-1

**InchiKey:** AMRTYTSGKDPNTI-PAQAUXNCSA-N

**Formula:** C35H64O2Si2

**SMILES:** C=C[Si](C)(C)OC1CCC2(C)C(C1)C(O[Si](C)(C)C=C)CC1C3CCC(C(C)CCCC(C)C)C3(C)C

**Mol. weight [g/mol]:** 573.05

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.26		Crippen Method
logp	10.349		Crippen Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529374&Units=SI>

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

**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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