5«alpha»-Cholestan-3«beta»,6«alpha»-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)16-14-1

InchiKey: AMRTYTSGKDPNTI-WPMNABSPSA-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)

Mol. weight [g/mol]: 573.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.26		Crippen Method
logp	10.349		Crippen Method
rinpol	3454.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529394&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.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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https://www.chemeo.com/cid/28-330-4/5-alpha-Cholestan-3-beta-6-alpha-diol-VDMS.pdf

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