

5-Cholesten-3-«beta»,27-diol-16-one, TMS

Inchi: InChI=1S/C36H68O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)34-33(39-42(11,12)13)24-3
InchiKey: YYJXVSSTRSRZBT-ZDBODOHGSA-N
Formula: C36H68O3Si3
SMILES: CC(CCCC(C)C1C(O[Si](C)(C)C)=CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)C
Mol. weight [g/mol]: 633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	11.035		Crippen Method
rinpol	3645.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177527&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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