

5-Cholestenic acid, 3-«beta»,7-«alpha»-diol, TMS

Inchi:	InChI=1S/C36H68O4Si3/c1-25(15-14-16-26(2)34(37)40-43(11,12)13)29-17-18-30-33-31
InchiKey:	FPKGLSJLFHDABN-BFMVBWRGSA-N
Formula:	C36H68O4Si3
SMILES:	CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C
Mol. weight [g/mol]:	649.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	10.436		Crippen Method
rinpol	3418.00		NIST Webbook
rinpol	3420.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R177601&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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<https://www.chemeo.com/cid/24-611-6/5-Cholestenic-acid-3-beta-7-alpha-diol-TMS.pdf>

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