

5-Cholesten-3-«beta»,27-diol-7-one, TMS

Other names:	27-Hydroxy-7-oxo-cholesterol, 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-
InchiKey:	ISXGQPKTFZXOKD-ZRSSOKGFSA-N
Formula:	C36H68O3Si3
SMILES:	CC(CCCC(C)C1CCC2C3=C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)
Mol. weight [g/mol]:	633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	11.179		Crippen Method
rinpol	3789.00		NIST Webbook
rinpol	3710.00		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=R177547&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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