

7«alpha»,27-Dihydroxy-4-cholesten-3-one, TMS

Other names:	4-Cholesten-7-«alpha»,27-diol-3-one, 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:	LVBALRWAXSVALG-RVUDJKPNSA-N
Formula:	C36H68O3Si3
SMILES:	CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C)
Mol. weight [g/mol]:	633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	11.035		Crippen Method
rinsol	3581.00		NIST Webbook
rinsol	3545.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R177418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-394-9/7-alpha-27-Dihydroxy-4-cholesten-3-one-TMS.pdf>

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