

(20S)-5«alpha»-cholestan-3«beta»,20,25-triol, TMS

Inchi:	InChI=1S/C36H72O3Si3/c1-33(2,38-41(9,10)11)22-15-23-36(5,39-42(12,13)14)32-19-18
InchiKey:	PVYWPROIHQWIBM-OPKUXVAVSA-N
Formula:	C36H72O3Si3
SMILES:	CC(C)(CCCC(C)(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)
Mol. weight [g/mol]:	637.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	11.276		Crippen Method
rinpol	3502.00		NIST Webbook
rinpol	3503.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R279633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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.cheméo.com/cid/63-970-5/20S-5-alpha-cholestan-3-beta-20-25-triol-TMS.pdf>

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