

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

<b>Inchi:</b>	InChI=1S/C36H70O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36)35)42-43-44
<b>InchiKey:</b>	ACPUMZZEKMSBSV-JTQVGFLKSA-N
<b>Formula:</b>	C36H70O5Si4
<b>SMILES:</b>	CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C1
<b>Mol. weight [g/mol]:</b>	695.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	10.240		Crippen Method
rinpol	3185.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R177483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R177483&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

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

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