

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

Inchi:	InChI=1S/C36H70O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36)35)31
InchiKey:	ACPUMZZEKMSBSV-ZKVVBUKYSА-N
Formula:	C36H70O5Si4
SMILES:	CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C1
Mol. weight [g/mol]:	695.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	10.240		Crippen Method
rinpol	3302.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177498&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/45-228-9/5-Cholenoic-acid-3-beta-7-beta-diol-TMS.pdf>

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