

5-Cholenoic acid, 3-«beta»,12-«alpha»-dihydroxy, methyl ester, TMS

Other names:	3-«beta»,12-«alpha»-Dihydroxy-5-cholenoic acid, MeTMS
Inchi:	InChI=1S/C31H56O4Si2/c1-21(11-16-29(32)33-4)25-14-15-26-24-13-12-22-19-23(34-36)27-31
InchiKey:	DCHCBDDKWVQOSX-QPLDZBMISA-N
Formula:	C31H56O4Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12
Mol. weight [g/mol]:	548.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.205		Crippen Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393249&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/13-690-1/5-Cholenoic-acid-3-beta-12-alpha-dihydroxy-methyl-ester-TMS.pdf>

Generated by Cheméo on 2025-12-05 15:54:40.936820537 +0000 UTC m=+4698278.466861191.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.