

Cholanic acid, 7«beta»,12«alpha»-dihydroxy, Me-TMS

Other names:	7«beta»,12«alpha»-Dihydroxy-5«beta»-cholanic acid, methyl ester, TMS
Inchi:	InChI=1S/C31H58O4Si2/c1-21(14-17-28(32)33-4)23-15-16-24-29-25(20-27(31(23,24)3)3
InchiKey:	WLOQXQFDQGTWNC-VBHCNTDPSA-N
Formula:	C31H58O4Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CCCCC4(C)C3CC(O[Si](C)(C)C)C12C
Mol. weight [g/mol]:	550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
ripol	3519.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R534331&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/70-538-7/Cholanic-acid-7-beta-12-alpha-dihydroxy-Me-TMS.pdf>

Generated by Cheméo on 2025-12-05 13:50:38.58912526 +0000 UTC m=+4690836.119165924.

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