

# 3-«alpha»,7-«alpha»-Dihydroxy-12-keto-5-«beta»-cholanoic acid, MeTMS

Other names:	3-«beta»-Cholanoic acid, 3-«alpha»,7-«alpha»-dihydroxy-12-one, methyl ester,
Inchi:	InChI=1S/C31H56O5Si2/c1-20(11-14-28(33)34-4)23-12-13-24-29-25(19-27(32)31(23,24)30)21-22
InchiKey:	RMBKMRQJJQQWMM-WCJNXPNSA-N
Formula:	C31H56O5Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(=O)C
Mol. weight [g/mol]:	564.94

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	7.464		Crippen Method
rinpola	3391.00		NIST Webbook
rinpola	3391.00		NIST Webbook
rinpola	3391.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R393209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R393209&amp;Units=SI</a>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/19-953-3/3-alpha-7-alpha-Dihydroxy-12-keto-5-beta-cholanoic-acid-MeTMS.pdf>

Generated by Cheméo on 2024-04-30 17:54:56.222577176 +0000 UTC m=+16788945.143154491.

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