

2-«beta»,3-«alpha»,7-«alpha»,12-«alpha»-Tetrahydroxy-5-beta-cholanoic acid, MeTMS methyl ester, TMS

Other names:	2-«beta»,3-«alpha»,7-«alpha»,12-«alpha»-tetrahydroxy-5-beta-cholanoic acid, MeTMS methyl ester, TMS
Inchi:	InChI=1S/C37H74O6Si4/c1-25(17-20-34(38)39-4)27-18-19-28-35-29(23-33(37(27,28)3)4
InchiKey:	MOHUSTFELXDKJF-LBHIDZRZSA-N
Formula:	C37H74O6Si4
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC4
Mol. weight [g/mol]:	727.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Crippen Method
logp	9.945		Crippen Method
rinpol	3440.00		NIST Webbook
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rinpol	3440.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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.chemeo.com/cid/57-064-8/2-beta-3-alpha-7-alpha-12-alpha-Tetrahydroxy-5-beta-cholanoic-acid-MeTMS>

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