

Murocholic acid, trimethyl ether-methyl ester

Other names:	3«alpha»,6«beta»-Dihydroxy-5«beta»-cholanoic acid, MeTMS 3«alpha»,6«beta»-Dihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
Inchi:	InChI=1S/C31H58O4Si2/c1-21(11-14-29(32)33-4)24-12-13-25-23-20-28(35-37(8,9)10)27
InchiKey:	FYDBJLGZNLQEL-HPRGHICTSA-N
Formula:	C31H58O4Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3242.00		NIST Webbook
rinpol	3268.00		NIST Webbook
rinpol	3242.00		NIST Webbook
rinpol	3242.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/63-517-8/Murocholic-acid-trimethyl-ether-methyl-ester.pdf>

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