

«DELTA»7-Lithocholic acid, trimethylsilyl ether-methyl ester

Other names:	3«alpha»-Hydroxy-«DELTA»7-5«beta» -cholanoic acid, MeTMS
Inchi:	InChI=1S/C28H48O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6
InchiKey:	WJIVWCYQOAJLNZ-UXUOZFMHSA-N
Formula:	C28H48O3Si
SMILES:	COC(=O)CCC(C)C1CCC2C3=CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	460.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	7.375		Crippen Method
rinpol	3177.00		NIST Webbook
rinpol	3186.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182262&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/48-299-8/DELTA-7-Lithocholic-acid-trimethylsilyl-ether-methyl-ester.pdf>

Generated by Cheméo on 2024-04-19 14:31:20.29452263 +0000 UTC m=+15826329.215099942.

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