3«alpha»,7«beta»,12«alpha»-Trihydroxy-5«beta»-c
acid, MeTMS

Other names:	Ursocholic acid, trimethylsilyl ether-methyl ester
Inchi:	InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3
InchiKey:	DQKFOBXAKZGIPX-FZGJARPISA-N
Formula:	C34H66O5Si3
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si]
Mol. weight [g/mol]:	639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/20-364-5/3-alpha-7-beta-12-alpha-Trihydroxy-5-beta-cholanoic-acid-MeTMS.pdf
Generated by Cheméo on 2024-04-27 08:32:02.109258246 +0000 UTC m=+16495971.029835561.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.