

3«alpha»,6«beta»,7«beta»-Trihydroxy-5«beta»-cholanoic acid, MeTMS

Other names:	3-«alpha»,6-«beta»,7-«beta»-Trihydroxy-5-«beta»-cholanoic acid, methyl ester-trimethylsilyl ether 3-«alpha»,6-«beta»,7-«beta»-Trihydroxy-5-«beta»-cholic acid, methyl ester, TMS «beta»-Muricholic acid, trimethyl ether-methyl ester 5-«beta»-Cholanoic acid, 3-«alpha»,6-«beta»,7-«beta»-trihydroxy, methyl ester, TMS
Inchi:	InChI=1S/C34H66O5Si3/c1-23(14-17-29(35)36-4)25-15-16-26-30-27(19-21-33(25,26)2)3
InchiKey:	MPBUWUAYSIDIDGN-ILZJCXJKSA-N
Formula:	C34H66O5Si3
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4
Mol. weight [g/mol]:	639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3348.00		NIST Webbook
rinpol	3374.00		NIST Webbook
rinpol	3348.00		NIST Webbook
rinpol	3321.00		NIST Webbook
rinpol	3348.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182222&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/46-349-4/3-alpha-6-beta-7-beta-Trihydroxy-5-beta-cholanoic-acid-MeTMS.pdf>

Generated by Cheméo on 2024-04-26 09:15:20.722291005 +0000 UTC m=+16412169.642868326.

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