

3-«alpha»-Trimethylsilyloxycholanolic acid, trimethylsilyl ester

Other names:	3«alpha»-hydroxy-5«beta»-cholan-24-oic acid, TMS
Inchi:	InChI=1S/C30H56O3Si2/c1-21(10-15-28(31)33-35(7,8)9)25-13-14-26-24-12-11-22-20-23
InchiKey:	PZEKZBLVDCPZQL-UHFFFAOYSA-N
Formula:	C30H56O3Si2
SMILES:	CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	520.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	8.660		Crippen Method
rinpol	3198.00		NIST Webbook
rinpol	3204.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U79234&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

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<https://www.chemeo.com/cid/64-419-6/3-alpha-Trimethylsilyloxycholanolic-acid-trimethylsilyl-ester.pdf>

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