

Cholest-5-en-7-one, 3-[(trimethylsilyl)oxy]-

Other names:	5-Cholesten-3«beta»-ol-7-one, trimethylsilyl ether 7-Ketocholesterol, tms derivative
Inchi:	InChI=1S/C30H52O2Si/c1-20(2)10-9-11-21(3)24-12-13-25-28-26(15-17-30(24,25)5)29(4
InchiKey:	SUBMBDZGNNFYKR-WAAFKJAVSA-N
Formula:	C30H52O2Si
SMILES:	CC(C)CCCC(C)C1CCC2C3C(=O)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	472.82
CAS:	55429-58-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	8.427		Crippen Method
rinpol	4363.60		NIST Webbook
rinpol	4431.80		NIST Webbook
rinpol	4363.60		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=C55429588&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.chemeo.com/cid/97-179-7/Cholest-5-en-7-one-3-trimethylsilyl-oxy.pdf>

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