

cis-5-Dodecenoic acid, trimethylsilyl ester

Other names:	5-Dodecenoic acid, (z)-, tms derivative
Inchi:	InChI=1S/C15H30O2Si/c1-5-6-7-8-9-10-11-12-13-14-15(16)17-18(2,3)4/h10-11H,5-9,12-
InchiKey:	MHKHFLVEYCFJDE-KHPPLWFESA-N
Formula:	C15H30O2Si
SMILES:	CCCCCCC=CCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	270.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	5.061		Crippen Method
rinpol	1625.60		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1625.60		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=U333637&Units=SI

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/50-212-0/cis-5-Dodecenoic-acid-trimethylsilyl-ester.pdf>

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