

cis-13-Eicosenoic acid, trimethylsilyl ester

Other names:	13-Eicosenoic acid, (z)-, tms derivative
Inchi:	InChI=1S/C23H46O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)25
InchiKey:	FJGSFFZFFXCMAF-KHPPLWFESA-N
Formula:	C23H46O2Si
SMILES:	CCCCCCC=CCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	382.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.22		Crippen Method
logp	8.182		Crippen Method
rinpol	2426.10		NIST Webbook
rinpol	2426.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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/58-042-1/cis-13-Eicosenoic-acid-trimethylsilyl-ester.pdf>

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