

(S)-(-)-Citronellic acid, trimethylsilyl ester

Other names:	(S)-(-)-citronellic acid, tms derivative
Inchi:	InChI=1S/C13H26O2Si/c1-11(2)8-7-9-12(3)10-13(14)15-16(4,5)6/h8,12H,7,9-10H2,1-6H
InchiKey:	NVBOIUPUPKAOBL-UHFFFAOYSA-N
Formula:	C13H26O2Si
SMILES:	CC(C)=CCCC(C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	242.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	4.137		Crippen Method
rinpol	1389.60		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333555&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/123-698-1/S-Citronellic-acid-trimethylsilyl-ester.pdf>

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