

# (S)-(-)-Citronellic acid, tert-butyldimethylsilyl ester

Other names:	(S)-(-)-citronellic acid, tbdms derivative
Inchi:	InChI=1S/C16H32O2Si/c1-13(2)10-9-11-14(3)12-15(17)18-19(7,8)16(4,5)6/h10,14H,9,11H
InchiKey:	PAYDULIHYPMYID-UHFFFAOYSA-N
Formula:	C16H32O2Si
SMILES:	CC(C)=CCCC(C)CC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	284.51

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	5.307		Crippen Method
rinpol	1618.70		NIST Webbook
rinpol	1618.70		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333554&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## 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/123-700-7/S-Citronellic-acid-tert-butyldimethylsilyl-ester.pdf>

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