«beta»-Citronellol, tert-butyldimethylsilyl ether

Other names:	tert-Butyl[(3,7-dimethyloct-6-en-1-yl)oxy]dimethylsilane
	«BETA»-citronellol, tbdms derivative
Inchi:	InChI=1S/C16H34OSi/c1-14(2)10-9-11-15(3)12-13-17-18(7,8)16(4,5)6/h10,15H,9,11-13H
InchiKey:	NFSXVFBFWBTHLM-UHFFFAOYSA-N
Formula:	C16H34OSi
SMILES:	CC(C)=CCCC(C)CCO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	270.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	5.781		Crippen Method
rinpol	1522.50		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333060&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices