

Linalool, trimethylsilyl ether

Other names:	Linalool, tms derivative
Inchi:	InChI=1S/C13H26OSi/c1-8-13(4,14-15(5,6)7)11-9-10-12(2)3/h8,10H,1,9,11H2,2-7H3
InchiKey:	GSRJPHNVKPGXHU-UHFFFAOYSA-N
Formula:	C13H26OSi
SMILES:	<chem>C=CC(C)(CCC=C(C)C)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	226.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	4.529		Crippen Method
rinpol	1227.40		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/90-810-2/Linalool-trimethylsilyl-ether.pdf>

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