

# 3-Methyl-2-butenyl (E)-caffeate, bis-TMS

<b>Other names:</b>	3-Methyl-2-butenyl (E)-caffeate, TMS 3-Methyl-2-butenyl caffeate, TMS
<b>Inchi:</b>	InChI=1S/C20H32O4Si2/c1-16(2)13-14-22-20(21)12-10-17-9-11-18(23-25(3,4)5)19(15-1
<b>InchiKey:</b>	VXQJJTOLIGXTFH-ZRDIBKRKSA-N
<b>Formula:</b>	C20H32O4Si2
<b>SMILES:</b>	CC(C)=CCOC(=O)C=Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
<b>Mol. weight [g/mol]:</b>	392.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	5.637		Crippen Method
rinpol	2422.00		NIST Webbook
rinpol	2396.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2422.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R55636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R55636&amp;Units=SI</a>

## Legend

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

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