

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

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	5.637		Crippen Method
rinpola	2383.00		NIST Webbook
rinpola	2390.00		NIST Webbook
rinpola	2383.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55622&Units=SI

Legend

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

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<https://www.chemeo.com/cid/53-521-4/2-Methyl-2-butenyl-E-caffeate-bis-TMS.pdf>

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