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

Other names: 3-Methyl-2-butenyl (E)-caffeate, TMS
3-Methyl-2-butenyl caffeate, TMS
Inchi: 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
InchiKey: VXQJJTOLIGXTFH-ZRDIBKRKSA-N
Formula: C20H32O4Si2
SMILES: CC(C)=CCOC(=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
rinpol	2422.00		NIST Webbook
rinpol	2396.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2422.00		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=R55636&Units=SI

Legend

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