

2-Propenoic acid, 3-[3,5-dimethoxy-4-[(trimethylsilyl)oxy]phenyl]-, trimethylsilyl ester, (E)-

Other names:	Trimethylsilyl (2E)-3-[3,5-dimethoxy-4-[(trimethylsilyl)oxy]phenyl]-2-propenoate Sinapic acid, bis-TMS, (E) Sinapic acid, TMS, (E) Sinapinic acid, (e)-, 2tms derivative
Inchi:	InChI=1S/C17H28O5Si2/c1-19-14-11-13(9-10-16(18)21-23(3,4)5)12-15(20-2)17(14)22-2
InchiKey:	LKLXWSPPLVNURP-MDZDMXLPSA-N
Formula:	C17H28O5Si2
SMILES:	COc1cc(C=CC(=O)O[Si](C)(C)C)cc(OC)c1O[Si](C)(C)C
Mol. weight [g/mol]:	368.57
CAS:	67460-48-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.13		Crippen Method
logp	4.309		Crippen Method

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=C67460484&Units=SI&Mask=3FFF

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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