

Cinnamic acid, 3,5-dimethoxy-4-(trimethylsiloxy)-, trimethylsilyl ester

Other names:	Cinnamic acid, 4-hydroxy-3,5-dimethoxy, bis-TMS Sinapic acid, bis-TMS Sinapic acid, TMS SINAPINIC ACID (2TMS) 2-Propenoic acid, 3-[3,5-dimethoxy-4-[(trimethylsilyl)oxy]phenyl]-, trimethylsilyl ester Trimethylsilyl 3-(3,5-dimethoxy-4-[(trimethylsilyl)oxy]phenyl)-2-propenoate Sinapinic acid, TMS (E)-Sinapic acid, TMS (Z)-Sinapic acid, TMS Sinapic acid, O,O'-di(trimethylsilyl)- Cinnamic acid, 3,5-dimethoxy-4-hydroxy, bis-TMS cis-Sinapic acid, TMS trans-Sinapic acid, TMS Sinapinic acid, 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:	27750-80-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.13		Crippen Method
logp	4.309		Crippen Method
rinpol	2267.00		NIST Webbook
rinpol	2272.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2257.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2261.00		NIST Webbook
rinpol	2242.20		NIST Webbook
rinpol	2259.00		NIST Webbook

rmpol	2275.00	NIST Webbook
rmpol	2259.00	NIST Webbook
rmpol	2273.00	NIST Webbook
rmpol	2261.00	NIST Webbook
rmpol	2257.00	NIST Webbook
rmpol	2249.00	NIST Webbook
rmpol	2273.00	NIST Webbook
rmpol	2249.00	NIST Webbook

Sources

Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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