

Trimethylsilyl 3-methoxy-4-(trimethylsilyloxy)cinnamate

Other names:	2-Propenoic acid, 3-[3-methoxy-4-[(trimethylsilyl)oxy]phenyl]-, trimethylsilyl ester Cinnamic acid, 3-methoxy-4-(trimethylsilyloxy)-, trimethylsilyl ester Cinnamic acid, 4-hydroxy-3-methoxy, bis-TMS Cinnamic acid, 4-hydroxy-3-methoxy, TMS Ferulic acid, TMS Ferulic acid, (2TMS) Ferulic acid, bis-TMS Ferulic acid, di-TMS Trimethylsilyl 3-(3-methoxy-4-[(trimethylsilyl)oxy]phenyl)-2-propenoate (E)-Ferulic acid, TMS (Z)-Ferulic acid, TMS Cinnamic acid, 3-methoxy-4-hydroxy, bis-TMS cis-Ferulic acid, TMS trans-Ferulic acid, TMS Ferulic acid, 2tms derivative
Inchi:	InChI=1S/C16H26O4Si2/c1-18-15-12-13(8-10-14(15)19-21(2,3)4)9-11-16(17)20-22(5,6)7
InchiKey:	UQBSUVIBJIXFQT-PKQBQFBNSA-N
Formula:	C16H26O4Si2
SMILES:	COc1cc(C=CC(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	338.55
CAS:	10517-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.01		Crippen Method
logp	4.300		Crippen Method
rinpol	2108.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2093.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2086.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2092.70		NIST Webbook

rinpol	2096.00	NIST Webbook
rinpol	2104.00	NIST Webbook
rinpol	2106.00	NIST Webbook
rinpol	2106.00	NIST Webbook
rinpol	2101.00	NIST Webbook
rinpol	2105.00	NIST Webbook
rinpol	2107.00	NIST Webbook
rinpol	2077.00	NIST Webbook
rinpol	2076.00	NIST Webbook
rinpol	2100.00	NIST Webbook
rinpol	2101.00	NIST Webbook
rinpol	2106.00	NIST Webbook
rinpol	2104.00	NIST Webbook
rinpol	2104.00	NIST Webbook
rinpol	2105.00	NIST Webbook
rinpol	2101.00	NIST Webbook
rinpol	2090.00	NIST Webbook
rinpol	2092.70	NIST Webbook
rinpol	2108.00	NIST Webbook
rinpol	2104.00	NIST Webbook
rinpol	2100.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10517096&Units=SI

Legend

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

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