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-(trimethylsiloxy)-, 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-PKNBQFBNSA-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/ci990307l

Crippen Method: https://www.chemeo.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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