

Trimethylsilyl 3,4-bis(trimethylsiloxy)cinnamate

Other names:

2-Propenoic acid, 3-[3,4-bis[(trimethylsilyl)oxy]phenyl]-, trimethylsilyl ester

Cinnamic acid, 3,4-bis(trimethylsiloxy)-, trimethylsilyl ester

Caffeic acid (tri-TMS)

Trimethylsilyl 3-(3,4-bis[(trimethylsilyl)oxy]phenyl)-2-propenoate

Trimethylsilyl 3,4-bis(trimethylsiloxy)caffeic acid

Caffeic acid (3TMS)

Caffeic acid, tris-TMS

Cinnamic acid, 3,4-dihydroxy, tri-TMS

Caffeic acid, TMS

Cinnamic acid, 3,4-dihydroxy, TMS

(Z)-Caffeic acid, TMS

Cinnamic acid, 3,4-dihydroxy, tris-TMS

Caffeic acid, 3tms derivative

Inchi:

InChI=1S/C18H32O4Si3/c1-23(2,3)20-16-12-10-15(14-17(16)21-24(4,5)6)11-13-18(19)2

InchiKey:

MBIYCWDFSLHMSI-ACCUITESSA-N

Formula:

C18H32O4Si3

SMILES:

C[Si](C)(C)OC(=O)C=Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1

Mol. weight [g/mol]:

396.70

CAS:

10586-03-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	5.505		Crippen Method
rinpol	2152.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2163.00		NIST Webbook
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2136.50		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2152.00		NIST Webbook

rropol	2158.00	NIST Webbook
rropol	2152.00	NIST Webbook
rropol	2158.00	NIST Webbook
rropol	2143.00	NIST Webbook
rropol	2141.00	NIST Webbook
rropol	2133.90	NIST Webbook
rropol	2151.00	NIST Webbook
rropol	2133.90	NIST Webbook
rropol	2155.00	NIST Webbook
rropol	2163.00	NIST Webbook
rropol	2136.50	NIST Webbook
rropol	2158.00	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=C10586035&Units=SI

Legend

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

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