

Cinnamic acid, p-(trimethylsiloxy)-, trimethylsilyl ester

Other names:

p-Coumaric acid (TMS)
Trimethylsilyl 3-(4-[(trimethylsilyl)oxy]phenyl)-2-propenoate
Cinnamic acid, 4-hydroxy, bis-TMS
p-Coumaric acid, di-TMS
p-Coumaric acid, bis-TMS
2-Propenoic acid, 3-[4-[(trimethylsilyl)oxy]phenyl]-, trimethylsilyl ester
(E)-p-Coumaric acid, TMS
p-Coumaric acid, di-TMS
p-COUMARIC ACID (2TMS)
Cinnamic acid, 4-hydroxy, TMS
(Z)-p-Coumaric acid, TMS
trans-p-Coumaric acid, TMS
cis-p-Coumaric acid, TMS
Di-p-Coumaric acid, TMS
p-Coumaric acid, TMS, (E)
4-Hydroxycinnamic acid, bis-TMS
4-Coumaric acid, 2tms derivative

Inchi:

InChI=1S/C15H24O3Si2/c1-19(2,3)17-14-10-7-13(8-11-14)9-12-15(16)18-20(4,5)6/h7-12

InchiKey:

RKLSIGFDXPECDB-FMIVXFBMSA-N

Formula:

C15H24O3Si2

SMILES:

C[Si](C)(C)OC(=O)C=Cc1ccc(O[Si](C)(C)C)cc1

Mol. weight [g/mol]:

308.52

CAS:

10517-30-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.11		Crippen Method
logp	4.292		Crippen Method
rinpol	1948.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1940.00		NIST Webbook

rinpol	1940.00	NIST Webbook
rinpol	1943.50	NIST Webbook
rinpol	1943.00	NIST Webbook
rinpol	1955.00	NIST Webbook
rinpol	1957.00	NIST Webbook
rinpol	1951.00	NIST Webbook
rinpol	1961.00	NIST Webbook
rinpol	1947.00	NIST Webbook
rinpol	1955.00	NIST Webbook
rinpol	1925.00	NIST Webbook
rinpol	1924.00	NIST Webbook
rinpol	1944.00	NIST Webbook
rinpol	1942.00	NIST Webbook
rinpol	1949.00	NIST Webbook
rinpol	1947.00	NIST Webbook
rinpol	1947.00	NIST Webbook
rinpol	1942.00	NIST Webbook

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=C10517303&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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