

trans-2,4-Dimethoxycinnamic acid, tert-butyldimethylsilyl ester

Other names:	2,4-Dimethoxycinnamic acid, (e)-, tbdms derivative
Inchi:	InChI=1S/C17H26O4Si/c1-17(2,3)22(6,7)21-16(18)11-9-13-8-10-14(19-4)12-15(13)20-5/
InchiKey:	BQAREBFODUFEEV-PKNCBQFBNSA-N
Formula:	C17H26O4Si
SMILES:	COc1ccc(C=CC(=O)O[Si](C)(C)C(C)(C)C)c(OC)c1
Mol. weight [g/mol]:	322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	4.265		Crippen Method
rinpol	2307.50		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=U352417&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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<https://www.chemeo.com/cid/22-594-8/trans-2-4-Dimethoxycinnamic-acid-tert-butyldimethylsilyl-ester.pdf>

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