

# Caffeic acid, O,O'-bis(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names:	Caffeic acid, TBDMS
Inchi:	InChI=1S/C27H50O4Si3/c1-25(2,3)32(10,11)29-22-18-16-21(20-23(22)30-33(12,13)26(4
InchiKey:	JQQURVFIEYNWDO-HTXNQAPBSA-N
Formula:	C27H50O4Si3
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)C=Cc1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	522.94
CAS:	180715-88-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	9.016		Crippen Method
rinpol	2848.70		NIST Webbook
rinpol	2865.00		NIST Webbook
rinpol	2848.70		NIST Webbook
rinpol	2865.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C180715882&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/55-354-8/Caffeic-acid-O-O-bis-tert-butyldimethylsilyl-tert-butyldimethylsilyl-ester.pdf>

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