(E)-Caffeic acid, TMS

Other names:	trans-Caffeic acid, triTMS
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)22
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:	67460-53-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	5.505		Crippen Method
rinpol	2144.00		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=C67460531&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/70-991-4/E-Caffeic-acid-TMS.pdf
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