

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

Other names:	Hydrocaffeic acid (3TMS) Trimethylsilyl 3-(3,4-bis[(trimethylsilyl)oxy]phenyl)propanoate 3,4-Dihydroxyhydrocinnamic acid, O,O-bis(trimethylsilyl)-, trimethylsilyl ester Benzenepropanoic acid, 3,4-bis-(trimethylsilyloxy), trimethylsilyl ester Phenylpropanoic acid, 3,4-dihydroxy, tris-TMS Phenylpropanoic acid, 3,4-dihydroxy, TMS 3,4-Dihydroxyhydrocinnamic acid, 3tms derivative
Inchi:	InChI=1S/C18H34O4Si3/c1-23(2,3)20-16-12-10-15(14-17(16)21-24(4,5)6)11-13-18(19)2
InchiKey:	DJVNRWQENHJMA-UHFFFAOYSA-N
Formula:	C18H34O4Si3
SMILES:	C[Si](C)(C)OC(=O)CCc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	398.72
CAS:	27750-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.12		Crippen Method
logp	5.425		Crippen Method
rinpol	1950.00		NIST Webbook
rinpol	1942.50		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1942.50		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750681&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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