

2-Propenoic acid, 3-phenyl-, trimethylsilyl ester

Other names:	Cinnamic acid, trimethylsilyl ester Cinnamic acid, TMS Trimethylsilyl 3-phenyl-2-propenoate (Z)-Cinnamic acid, TMS (E)-Cinnamic acid, TMS Cinnamic acid, tms derivative
Inchi:	InChI=1S/C12H16O2Si/c1-15(2,3)14-12(13)10-9-11-7-5-4-6-8-11/h4-10H,1-3H3
InchiKey:	HEVXLPBSUCJVAQ-UHFFFAOYSA-N
Formula:	C12H16O2Si
SMILES:	<chem>C[Si](C)(C)OC(=O)C=Cc1ccccc1</chem>
Mol. weight [g/mol]:	220.34
CAS:	2078-20-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	3.078		Crippen Method
rinpol	1540.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1526.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078208&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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