

2-Propenoic acid, 3-phenyl-, trimethylsilyl ester, (E)-

Other names:	Trimethylsilyl (2E)-3-phenyl-2-propenoate (E)-Cinnamic acid, TMS trans-Cinnamic acid, TMS trans-Cinnamic acid, trimethylsilyl ester Cinnamic acid, (e)-, 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/b10-9+
InchiKey:	HEVXLPBSUCJVAQ-MDZDMXLPSA-N
Formula:	C12H16O2Si
SMILES:	C[Si](C)(C)OC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	220.34
CAS:	55012-82-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	3.078		Crippen Method
rinpol	1514.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1555.40		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1547.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55012823&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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