Benzenepropanoic acid, trimethylsilyl ester

Other names:	Hydrocinnamic acid, trimethylsilyl ester
	Trimethylsilyl 3-phenylpropanoate
	Dihydrocinnamic acid, TMS
	Dihydrocinnamic (benzenepropanoic) acid, TMS
	Benzenepropanoic acid, tms derivative
Inchi:	InChI=1S/C12H18O2Si/c1-15(2,3)14-12(13)10-9-11-7-5-4-6-8-11/h4-8H,9-10H2,1-3H3
InchiKey:	GRONVOGSDOJOMG-UHFFFAOYSA-N
Formula:	C12H18O2Si
SMILES:	C[Si](C)(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]:	222.36
CAS:	21273-15-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	2.997		Crippen Method
rinpol	1414.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1414.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21273154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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