(.+/-.)-2-Phenylbutyric acid, trimethylsilyl ester

Other names:	Trimethylsilyl 2-phenylbutanoate
	Butanoic acid, 2-phenyl, mono-TMS
	Butanoic acid, 2-phenyl, TMS
	Butanoic acid, 2-phenyl, trimethylsilyl ester
	2-Phenylbutyric acid, tms derivative
Inchi:	InChI=1S/C13H20O2Si/c1-5-12(11-9-7-6-8-10-11)13(14)15-16(2,3)4/h6-10,12H,5H2,1-4H
InchiKey:	VYKUZPWIVBWKQA-UHFFFAOYSA-N
Formula:	C13H20O2Si
SMILES:	CCC(C(=O)O[Si](C)(C)C)c1ccccc1
Mol. weight [g/mol]:	236.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	3.558		Crippen Method
rinpol	1359.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1382.60		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1378.80		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1378.80		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=U332775&Units=SI

Legend

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