Benzenepropanoic acid, tert-butyldimethylsilyl ester

Other names:	3-Phenylpropionic acid, TBDMS
Inchi:	InChI=1S/C15H24O2Si/c1-15(2,3)18(4,5)17-14(16)12-11-13-9-7-6-8-10-13/h6-10H,11-12
InchiKey:	DMEANXAVVZKYTA-UHFFFAOYSA-N
Formula:	C15H24O2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]:	264.44
CAS:	78324-01-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	4.168		Crippen Method
rinpol	1653.00		NIST Webbook
rinpol	1653.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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