(.+/-.)-2-Phenylbutyric acid, dimethyl(3,3,3-trifluoropropyl)silyl ester

Inchi: InChI=1S/C15H21F3O2Si/c1-4-13(12-8-6-5-7-9-12)14(19)20-21(2,3)11-10-15(16,17)18/h

InchiKey: XRJNFNCFWQMMJZ-UHFFFAOYSA-N

Formula: C15H21F3O2Si

SMILES: CCC(C(=O)O[Si](C)(C)CCC(F)(F)F)c1ccccc1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	4.881		Crippen Method
rinpol	1485.00		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=U375600&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices