

(.+/-)-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)CC(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.cheméo.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

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