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

Inchi: InChI=1S/C13H19BrO2Si/c1-4-12(11-8-6-5-7-9-11)13(15)16-17(2,3)10-14/h5-9,12H,4,10

InchiKey: VIBWUUIMODRAIZ-UHFFFAOYSA-N

Formula: C13H19BrO2Si

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

Mol. weight [g/mol]: 315.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	3.863		Crippen Method
rinpol	1697.00		NIST Webbook
rinpol	1697.00		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=U375606&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices