(.+/-.)-2-Phenylbutyric acid, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl 2-phenylbutanoate
2-Phenylbutyric acid, TBDMS
2-Phenylbutyric acid, tbdms derivative

Inchi: InChI=1S/C16H26O2Si/c1-7-14(13-11-9-8-10-12-13)15(17)18-19(5,6)16(2,3)4/h8-12,14H

InchiKey: IWSNKTSLOBHITP-UHFFFAOYSA-N

Formula: C16H26O2Si

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

Mol. weight [g/mol]: 278.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	4.729		Crippen Method
rinpol	1600.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1602.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333146&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices