3-Phenylbutyric acid, TBDMS

Inchi: InChI=1S/C16H26O2Si/c1-13(14-10-8-7-9-11-14)12-15(17)18-19(5,6)16(2,3)4/h7-11,13H
InchiKey: JDKNNBZVVUJDRI-UHFFFAOYSA-N
Formula: C16H26O2Si
SMILES: CC(CC(=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	1677.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563601&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