3-Phenoxypropionic acid, TBDMS

Inchi: InChI=1S/C21H28O3Si/c1-21(2,3)25(4,5)24-20(22)15-14-17-10-9-13-19(16-17)23-18-11-
InchiKey: IFIOMBICNDCWQO-UHFFFAOYSA-N
Formula: C21H28O3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 356.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	5.960		Crippen Method
rinpol	1774.00		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=R563592&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices