Phenylpropiolic acid, DMTBS

Other names: Phenylpropiolic acid, TBDMS
Inchi: InChI=1S/C15H20O2Si/c1-15(2,3)18(4,5)17-14(16)12-11-13-9-7-6-8-10-13/h6-10H,1-5H
InchiKey: VGXJNGONHYFIAL-UHFFFAOYSA-N
Formula: C15H20O2Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C#Cc1ccccc1
Mol. weight [g/mol]: 260.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	3.586		Crippen Method
rinpol	1772.00		NIST Webbook
rinpol	1775.00		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=R538586&Units=SI

Legend

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