Benzeneacetic acid, «alpha»-oxo-, trimethylsilyl ester

Other names: Benzoylformic acid TMS
Benzoylformic acid, mono-TMS
Phenylglyoxylic acid, tms derivative

Inchi: InChI=1S/C11H14O3Si/c1-15(2,3)14-11(13)10(12)9-7-5-4-6-8-9/h4-8H,1-3H3

InchiKey: IZVHGWPJDQCENH-UHFFFAOYSA-N

Formula: C11H14O3Si

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

Mol. weight [g/mol]: 222.31

CAS: 55517-36-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.30		Crippen Method
logp	2.247		Crippen Method
rinpol	1459.00		NIST Webbook
rinpol	1459.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517367&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