

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:	IZVHGWPDQJQCENH-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

Latest version available from:

<https://www.chemeo.com/cid/15-260-6/Benzeneacetic-acid-alpha-oxo-trimethylsilyl-ester.pdf>

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