

Benzeneacetic acid, trimethylsilyl ester

Other names:	Acetic acid, phenyl-, trimethylsilyl ester Trimethylsilyl phenylacetate Phenylacetic acid, monoTMS Phenylacetic acid, trimethylsilyl ester Benzeneacetic acid, tms derivative
Inchi:	InChI=1S/C11H16O2Si/c1-14(2,3)13-11(12)9-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey:	WWCXSUHALKENOU-UHFFFAOYSA-N
Formula:	C11H16O2Si
SMILES:	C[Si](C)(C)OC(=O)Cc1ccccc1
Mol. weight [g/mol]:	208.33
CAS:	2078-18-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.44		Crippen Method
logp	2.607		Crippen Method
rinpol	1301.60		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1295.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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