

Benzeneacetic acid, 2-methoxy-, trimethylsilyl ester

Other names:	2-Methoxyphenylacetic acid, tms derivative
Inchi:	InChI=1S/C12H18O3Si/c1-14-11-8-6-5-7-10(11)9-12(13)15-16(2,3)4/h5-8H,9H2,1-4H3
InchiKey:	RKCAHERJDCJFCL-UHFFFAOYSA-N
Formula:	C12H18O3Si
SMILES:	COc1ccccc1CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	238.35
CAS:	55590-71-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Crippen Method
logp	2.616		Crippen Method
rinpol	1476.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55590711&Units=SI

Legend

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

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<https://www.chemeo.com/cid/22-968-3/Benzeneacetic-acid-2-methoxy-trimethylsilyl-ester.pdf>

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