

Benzeneacetic acid, 4-methoxy-, trimethylsilyl ester

Other names:	Acetic acid, (p-methoxyphenyl)-, trimethylsilyl ester 4-Methoxybenzeneacetic acid, tms derivative
Inchi:	InChI=1S/C12H18O3Si/c1-14-11-7-5-10(6-8-11)9-12(13)15-16(2,3)4/h5-8H,9H2,1-4H3
InchiKey:	AHCNMCIDHXSNAK-UHFFFAOYSA-N
Formula:	C12H18O3Si
SMILES:	COc1ccc(CC(=O)O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	238.35
CAS:	27750-50-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Crippen Method
logp	2.616		Crippen Method
rinpol	1521.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750501&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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