

# Benzoic acid, 3-methoxy-, trimethylsilyl ester

<b>Other names:</b>	Benzoic acid, 3-methoxy, TMS
<b>Inchi:</b>	InChI=1S/C11H16O3Si/c1-13-10-7-5-6-9(8-10)11(12)14-15(2,3)4/h5-8H,1-4H3
<b>InchiKey:</b>	PPUSJGXNIQTKKU-UHFFFAOYSA-N
<b>Formula:</b>	C11H16O3Si
<b>SMILES:</b>	COc1cccc(C(=O)O[Si](C)(C)C)c1
<b>Mol. weight [g/mol]:</b>	224.33
<b>CAS:</b>	959111-51-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	2.687		Crippen Method
rinpol	1485.00		NIST Webbook
rinpol	1455.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C959111514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C959111514&amp;Units=SI</a>

## Legend

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

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