

# Benzoic acid, 4-chloro-, trimethylsilyl ester

<b>Other names:</b>	Benzoic acid, p-chloro-, trimethylsilyl ester Trimethylsilyl ester of 4-Chlorobenzoic acid 4-Chlorobenzoic acid, tms derivative
<b>Inchi:</b>	InChI=1S/C10H13ClO2Si/c1-14(2,3)13-10(12)8-4-6-9(11)7-5-8/h4-7H,1-3H3
<b>InchiKey:</b>	XGABXNUFKZKQCO-UHFFFAOYSA-N
<b>Formula:</b>	C10H13ClO2Si
<b>SMILES:</b>	C[Si](C)(C)OC(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	228.75
<b>CAS:</b>	25436-27-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	3.332		Crippen Method
rinpol	1388.00		NIST Webbook
rinpol	1414.50		NIST Webbook

## Sources

<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=C25436275&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25436275&amp;Units=SI</a>
<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>

## 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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