

3-Chlorobenzoic acid, trimethylsilyl ester

Other names:	Benzoic acid, 3-chloro, trimethylsilyl ester Trimethylsilyl 3-chlorobenzoate m-Chlorobenzoic acid, trimethylsilyl ester derivative 3-Chlorobenzoic acid, tms derivative
Inchi:	InChI=1S/C10H13ClO2Si/c1-14(2,3)13-10(12)8-5-4-6-9(11)7-8/h4-7H,1-3H3
InchiKey:	APACGNWFQWQPTA-UHFFFAOYSA-N
Formula:	C10H13ClO2Si
SMILES:	C[Si](C)(C)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	228.75
CAS:	114521-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	3.332		Crippen Method
rinpol	1385.00		NIST Webbook
rinpol	1385.00		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=C114521538&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/115-692-6/3-Chlorobenzoic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-27 18:49:05.946416386 +0000 UTC m=+16532994.866993707.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.