

Imidazole, 1-(m-chlorophenyl)-

Other names:	1-(m-Chlorophenyl)imidazole 1H-Imidazole, 1-(3-chlorophenyl)-
Inchi:	InChI=1S/C9H7ClN2/c10-8-2-1-3-9(6-8)12-5-4-11-7-12/h1-7H
InchiKey:	LEKTXVRARNYCNV-UHFFFAOYSA-N
Formula:	C9H7ClN2
SMILES:	<chem>Clc1cccc(-n2ccnc2)c1</chem>
Mol. weight [g/mol]:	178.62
CAS:	51581-52-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.526		Crippen Method
mvol	126.650	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51581523&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/33-910-4/Imidazole-1-m-chlorophenyl.pdf>

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