

1-(4-Chlorophenyl)imidazole

Inchi:	InChI=1S/C9H7CIN2/c10-8-1-3-9(4-2-8)12-6-5-11-7-12/h1-7H
InchiKey:	BARLRKAYTDVUIS-UHFFFAOYSA-N
Formula:	C9H7CIN2
SMILES:	Clc1ccc(-n2ccnc2)cc1
Mol. weight [g/mol]:	178.62
CAS:	51581-54-5

Physical Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51581545&Units=SI
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

Legend

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

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<https://www.chemeo.com/cid/11-300-5/1-4-Chlorophenyl-imidazole.pdf>

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