

1-(2-Chlorophenyl)imidazoline-2-thione

Other names:	Imidazole-2-thione, 1-(2-chlorophenyl)-
Inchi:	InChI=1S/C9H7ClN2S/c10-7-3-1-2-4-8(7)12-6-5-11-9(12)13/h1-6H,(H,11,13)
InchiKey:	XOCLHGYTLWVXQB-UHFFFAOYSA-N
Formula:	C9H7ClN2S
SMILES:	Sc1nccn1-c1ccccc1Cl
Mol. weight [g/mol]:	210.68
CAS:	51581-47-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.09		Crippen Method
logp	2.814		Crippen Method
mcvol	143.000	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51581476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/32-934-9/1-2-Chlorophenyl-imidazoline-2-thione.pdf>

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