

2-Chloro-5-methoxybenzimidazole

Inchi:	InChI=1S/C8H7ClN2O/c1-12-5-2-3-6-7(4-5)11-8(9)10-6/h2-4H,1H3,(H,10,11)
InchiKey:	FMDGYQOERIOABX-UHFFFAOYSA-N
Formula:	C8H7ClN2O
SMILES:	<chem>COc1ccc2[nH]c(Cl)nc2c1</chem>
Mol. weight [g/mol]:	182.61
CAS:	15965-54-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	1.743		Crippen Method
mcvol	122.730	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=C15965545&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/22-502-9/2-Chloro-5-methoxybenzimidazole.pdf>

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