

Benzimidazole, 5-chloro-2-methyl-1-phenyl-

Other names:	5-chloro-2-methyl-1-phenyl-1H-benzimidazole
Inchi:	InChI=1S/C14H11ClN2/c1-10-16-13-9-11(15)7-8-14(13)17(10)12-5-3-2-4-6-12/h2-9H,1H
InchiKey:	BDYHHBOQBZEHLL-UHFFFAOYSA-N
Formula:	C14H11ClN2
SMILES:	<chem>Cc1nc2cc(Cl)ccc2n1-c1ccccc1</chem>
Mol. weight [g/mol]:	242.70
CAS:	84100-59-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	3.987		Crippen Method
mcvol	177.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84100594&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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