

5-Chloro-benzofurazan

Other names:	5-chlorobenzofurazan
Inchi:	InChI=1S/C6H3ClN2O/c7-4-1-2-5-6(3-4)9-10-8-5/h1-3H
InchiKey:	DGGUUSPCQWWLRM-UHFFFAOYSA-N
Formula:	C6H3ClN2O
SMILES:	Clc1ccc2nonc2c1
Mol. weight [g/mol]:	154.55
CAS:	19155-86-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.23		Crippen Method
logp	1.876		Crippen Method
mcvol	94.550	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=C19155863&Units=SI

Legend

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

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