

6-Chlorobenzofuroxan

Other names:	5-chlorobenzofuroxan
Inchi:	InChI=1S/C6H3ClN2O2/c7-4-1-2-5-6(3-4)9(10)11-8-5/h1-3H
InchiKey:	CVHOKJCSOAHYAJ-UHFFFAOYSA-N
Formula:	C6H3ClN2O2
SMILES:	[O-][n+]1onc2ccc(Cl)cc21
Mol. weight [g/mol]:	170.55
CAS:	39060-31-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.99		Crippen Method
logp	1.115		Crippen Method
mcvol	100.420	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=C39060316&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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