

2-Chloro-5-nitropyridine

Other names:	Pyridine, 2-chloro-5-nitro-
Inchi:	InChI=1S/C5H3ClN2O2/c6-5-2-1-4(3-7-5)8(9)10/h1-3H
InchiKey:	BAZVFQBTJPBRTJ-UHFFFAOYSA-N
Formula:	C5H3ClN2O2
SMILES:	O=[N+]([O-])c1ccc(Cl)nc1
Mol. weight [g/mol]:	158.54
CAS:	4548-45-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.643		Crippen Method
mcvol	97.190	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=C4548452&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/36-521-3/2-Chloro-5-nitropyridine.pdf>

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