

Pyrrolidine, 1-(5-chloro-2-nitrophenyl)

Inchi:	InChI=1S/C10H11ClN2O2/c11-8-3-4-9(13(14)15)10(7-8)12-5-1-2-6-12/h3-4,7H,1-2,5-6H
InchiKey:	NPIPVCGYGYIXQG-UHFFFAOYSA-N
Formula:	C10H11ClN2O2
SMILES:	O=[N+]([O-])c1ccc(Cl)cc1N1CCCC1
Mol. weight [g/mol]:	226.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.848		Crippen Method
mcvol	156.780	ml/mol	McGowan Method
rinpol	1912.00		NIST Webbook

Sources

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=R329545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/68-162-7/Pyrrolidine-1-5-chloro-2-nitrophenyl.pdf>

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