

Pyrrolidine, 1-(2-chloro-4-nitrophenyl)

Other names:	1-(2-chloro-4-nitrophenyl)pyrrolidine
Inchi:	InChI=1S/C10H11ClN2O2/c11-9-7-8(13(14)15)3-4-10(9)12-5-1-2-6-12/h3-4,7H,1-2,5-6H2
InchiKey:	XMLGZIMCJDYHOD-UHFFFAOYSA-N
Formula:	C10H11ClN2O2
SMILES:	O=[N+]([O-])c1ccc(N2CCCC2)c(Cl)c1
Mol. weight [g/mol]:	226.66
CAS:	55403-91-3

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	1930.00		NIST Webbook
rinpol	1930.00		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=C55403913&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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