

# N-[4-Chloro-2-nitrophenyl]pyrrolidine

**Other names:** Pyrrolidine, 1-(4-chloro-2-nitrophenyl)  
**Inchi:** InChI=1S/C10H11ClN2O2/c11-8-3-4-9(10(7-8)13(14)15)12-5-1-2-6-12/h3-4,7H,1-2,5-6H  
**InchiKey:** QATZMIJXHKOELL-UHFFFAOYSA-N  
**Formula:** C10H11ClN2O2  
**SMILES:** O=[N+]([O-])c1cc(Cl)ccc1N1CCCC1  
**Mol. weight [g/mol]:** 226.66  
**CAS:** 41173-36-8

## 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        | 1934.00 |        | NIST Webbook   |
| rinpol        | 1934.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C41173368&Units=SI>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/121-381-4/N-4-Chloro-2-nitrophenyl-pyrrolidine.pdf>

Generated by Cheméo on 2024-12-10 20:06:34.463406457 +0000 UTC m=+8442057.100375704.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.