

# 4-Chlorobenzoic acid, morpholide

**Inchi:** InChI=1S/C11H12ClNO2/c12-10-3-1-9(2-4-10)11(14)13-5-7-15-8-6-13/h1-4H,5-8H2  
**InchiKey:** BGRFQNTYHMHVFJ-UHFFFAOYSA-N  
**Formula:** C11H12ClNO2  
**SMILES:** O=C(c1ccc(Cl)cc1)N1CCOCC1  
**Mol. weight [g/mol]:** 225.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.812		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307393&Units=SI>  
**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)

## 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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