

# 7-Chlorocoumarin

**Inchi:** InChI=1S/C9H5ClO2/c10-7-3-1-6-2-4-9(11)12-8(6)5-7/h1-5H  
**InchiKey:** BWPNKJCEDYRUCB-UHFFFAOYSA-N  
**Formula:** C<sub>9</sub>H<sub>5</sub>ClO<sub>2</sub>  
**SMILES:** O=c1ccc2ccc(Cl)cc2o1  
**Mol. weight [g/mol]:** 180.59

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	2.446		Crippen Method
mcvol	118.430	ml/mol	McGowan Method
rinpol	1586.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1586.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R274292&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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

Latest version available from:

<https://www.cheméo.com/cid/69-433-5/7-Chlorocoumarin.pdf>

Generated by Cheméo on 2024-04-27 14:38:36.118404989 +0000 UTC m=+16517965.038982304.

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