

# 2-Chloro-4-methylphenyl isothiocyanate

**Inchi:** InChI=1S/C8H6CINS/c1-6-2-3-8(10-5-11)7(9)4-6/h2-4H,1H3  
**InchiKey:** UIZZXGXTVVWRED-UHFFFAOYSA-N  
**Formula:** C8H6CINS  
**SMILES:** Cc1ccc(N=C=S)c(Cl)c1  
**Mol. weight [g/mol]:** 183.66  
**CAS:** 57878-93-0

## Physical Properties

Property code	Value	Unit	Source
hf	273.47	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.383		Crippen Method
mvol	129.790	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	602.46	K	Joback Method
tc	868.07	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57878930&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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