

# Benzene, 4-chloro-1-isothiocyanato-2-methyl-

<b>Other names:</b>	3-chloro-6-isothiocyanatotoluene
<b>Inchi:</b>	InChI=1S/C8H6ClNS/c1-6-4-7(9)2-3-8(6)10-5-11/h2-4H,1H3
<b>InchiKey:</b>	XYTLRVPBHRTMS-UHFFFAOYSA-N
<b>Formula:</b>	C8H6ClNS
<b>SMILES:</b>	<chem>Cc1cc(Cl)ccc1N=C=S</chem>
<b>Mol. weight [g/mol]:</b>	183.66
<b>CAS:</b>	23165-53-9

## 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
mcvol	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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23165539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23165539&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	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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