

# Benzene, 1-chloro-2-(isothiocyanatomethyl)-

<b>Other names:</b>	Isothiocyanic acid, o-chlorobenzyl ester 2-Chlorobenzyl isothiocyanate
<b>Inchi:</b>	InChI=1S/C8H6CINS/c9-8-4-2-1-3-7(8)5-10-6-11/h1-4H,5H2
<b>InchiKey:</b>	RMVDNJDSLXQPAV-UHFFFAOYSA-N
<b>Formula:</b>	C8H6CINS
<b>SMILES:</b>	S=C=NCc1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	183.66
<b>CAS:</b>	18967-44-7

## Physical Properties

Property code	Value	Unit	Source
hf	284.94	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.943		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	597.48	K	Joback Method
tc	862.02	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=C18967447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18967447&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

hf: Enthalpy of formation at standard conditions

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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