

# Benzenethiol, 2-chloro-

<b>Other names:</b>	Benzenethiol, o-chloro- o-Chlorobenzenethiol o-Chloromercaptobenzene o-Chlorothiophenol 2-Chlorobenzenethiol 2-Chlorothiophenol
<b>Inchi:</b>	InChI=1S/C6H5ClS/c7-5-3-1-2-4-6(5)8/h1-4,8H
<b>InchiKey:</b>	PWOBDMNCYMQTCE-UHFFFAOYSA-N
<b>Formula:</b>	C6H5ClS
<b>SMILES:</b>	Sc1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	144.62
<b>CAS:</b>	6320-03-2

## Physical Properties

Property code	Value	Unit	Source
gf	119.88	kJ/mol	Joback Method
hf	80.63	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	43.01	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.629		Crippen Method
mcvol	100.230	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
tb	478.70	K	NIST Webbook
tc	720.14	K	Joback Method
tf	262.70	K	Joback Method
vc	0.366	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.41	J/mol×K	468.63	Joback Method
cpg	174.66	J/mol×K	510.55	Joback Method
cpg	183.22	J/mol×K	552.47	Joback Method

cpg	191.14	J/mol×K	594.38	Joback Method
cpg	198.44	J/mol×K	636.30	Joback Method
cpg	205.16	J/mol×K	678.22	Joback Method
cpg	211.34	J/mol×K	720.14	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	478.70	K	34.70	NIST Webbook

## 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=C6320032&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6320032&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>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion 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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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