

# 4-Chlorothiobenzamide

<b>Other names:</b>	p-Chlorobenzothiamide p-Chlorothiobenzamide Benzamide, p-chlorothio- Benzenecarbothioamide, 4-chloro-
<b>Inchi:</b>	InChI=1S/C7H6CINS/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H2,9,10)
<b>InchiKey:</b>	OKPUICCJRDBRJT-UHFFFAOYSA-N
<b>Formula:</b>	C7H6CINS
<b>SMILES:</b>	NC(=S)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	171.65
<b>CAS:</b>	2521-24-6

## Physical Properties

Property code	Value	Unit	Source
gf	282.42	kJ/mol	Joback Method
hf	201.80	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.974		Crippen Method
mcvol	120.000	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	571.22	K	Joback Method
tc	833.59	K	Joback Method
tf	355.04	K	Joback Method
vc	0.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.81	J/molxK	571.22	Joback Method
cpg	243.97	J/molxK	614.95	Joback Method
cpg	252.25	J/molxK	658.68	Joback Method
cpg	259.76	J/molxK	702.40	Joback Method
cpg	266.59	J/molxK	746.13	Joback Method

cpg	272.84	J/mol×K	789.86	Joback Method
cpg	278.62	J/mol×K	833.59	Joback Method

## Sources

<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=C2521246&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2521246&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>
<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>

## 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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