

# 4-Chloro-2-nitrobenzoic acid

<b>Other names:</b>	Benzoic acid, 4-chloro-2-nitro- 2-Nitro-4-chlorobenzoic acid
<b>Inchi:</b>	InChI=1S/C7H4ClNO4/c8-4-1-2-5(7(10)11)6(3-4)9(12)13/h1-3H,(H,10,11)
<b>InchiKey:</b>	JAHIPDTWWVYVRV-UHFFFAOYSA-N
<b>Formula:</b>	C7H4ClNO4
<b>SMILES:</b>	O=C(O)c1ccc(Cl)cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	201.56
<b>CAS:</b>	6280-88-2

## Physical Properties

Property code	Value	Unit	Source
gf	-140.91	kJ/mol	Joback Method
hf	-265.53	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.946		Crippen Method
mvol	122.830	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	731.52	K	Joback Method
tc	968.96	K	Joback Method
tf	504.39	K	Joback Method
vc	0.475	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.94	J/mol×K	731.52	Joback Method
cpg	290.51	J/mol×K	771.09	Joback Method
cpg	296.51	J/mol×K	810.67	Joback Method
cpg	301.95	J/mol×K	850.24	Joback Method
cpg	306.87	J/mol×K	889.81	Joback Method
cpg	311.30	J/mol×K	929.39	Joback Method
cpg	315.25	J/mol×K	968.96	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C6280882&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6280882&amp;Units=SI</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>h vap:</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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