

# Benzoic acid, 2-amino-5-chloro-

<b>Other names:</b>	Anthranilic acid, 5-chloro- 2-Amino-5-chlorobenzoic acid 5-Chloro-2-aminobenzoic acid 5-Chloroanthranilic acid
<b>Inchi:</b>	InChI=1S/C7H6ClNO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H,10,11)
<b>InchiKey:</b>	IFXKXCLVKQVVDI-UHFFFAOYSA-N
<b>Formula:</b>	C7H6ClNO2
<b>SMILES:</b>	<chem>Nc1ccc(Cl)cc1C(=O)O</chem>
<b>Mol. weight [g/mol]:</b>	171.58
<b>CAS:</b>	635-21-2

## Physical Properties

Property code	Value	Unit	Source
gf	-110.01	kJ/mol	Joback Method
hf	-220.98	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.620		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	652.21	K	Joback Method
tc	875.53	K	Joback Method
tf	444.04	K	Joback Method
vc	0.422	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.90	J/molxK	652.21	Joback Method
cpg	265.20	J/molxK	689.43	Joback Method
cpg	271.97	J/molxK	726.65	Joback Method
cpg	278.24	J/molxK	763.87	Joback Method
cpg	284.04	J/molxK	801.09	Joback Method

cpg	289.38	J/mol×K	838.31	Joback Method
cpg	294.28	J/mol×K	875.53	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.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=C635212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C635212&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>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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