

# Aniline, 2-bromo-3-chloro

<b>Inchi:</b>	InChI=1S/C6H5BrClN/c7-6-4(8)2-1-3-5(6)9/h1-3H,9H2
<b>InchiKey:</b>	JHHMLFBYFNAPDZ-UHFFFAOYSA-N
<b>Formula:</b>	C6H5BrClN
<b>SMILES:</b>	Nc1cccc(Cl)c1Br
<b>Mol. weight [g/mol]:</b>	206.47

## Physical Properties

Property code	Value	Unit	Source
gf	161.63	kJ/mol	Joback Method
hf	90.80	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.685		Crippen Method
mcvol	111.360	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
tb	549.44	K	Joback Method
tc	805.41	K	Joback Method
tf	381.82	K	Joback Method
vc	0.404	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.79	J/molxK	549.44	Joback Method
cpg	206.83	J/molxK	592.10	Joback Method
cpg	214.23	J/molxK	634.76	Joback Method
cpg	221.04	J/molxK	677.42	Joback Method
cpg	227.30	J/molxK	720.08	Joback Method
cpg	233.04	J/molxK	762.74	Joback Method
cpg	238.31	J/molxK	805.41	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=R621668&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R621668&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>mccvol:</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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