

# 4-Bromo-2-chlorobenzoic acid

<b>Other names:</b>	Benzoic acid, 4-bromo-2-chloro-
<b>Inchi:</b>	InChI=1S/C7H4BrClO2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,(H,10,11)
<b>InchiKey:</b>	JAVZWSOFJKYSDY-UHFFFAOYSA-N
<b>Formula:</b>	C7H4BrClO2
<b>SMILES:</b>	O=C(O)c1ccc(Br)cc1Cl
<b>Mol. weight [g/mol]:</b>	235.46
<b>CAS:</b>	59748-90-2

## Physical Properties

Property code	Value	Unit	Source
gf	-162.14	kJ/mol	Joback Method
hf	-228.44	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.801		Crippen Method
mcvol	122.910	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	645.84	K	Joback Method
tc	874.04	K	Joback Method
tf	420.58	K	Joback Method
vc	0.456	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.54	J/molxK	645.84	Joback Method
cpg	243.93	J/molxK	683.87	Joback Method
cpg	249.82	J/molxK	721.91	Joback Method
cpg	255.26	J/molxK	759.94	Joback Method
cpg	260.27	J/molxK	797.98	Joback Method
cpg	264.88	J/molxK	836.01	Joback Method
cpg	269.11	J/molxK	874.04	Joback Method
dvisc	0.0015492	Paxs	420.58	Joback Method

dvisc	0.0008109	Paxs	458.12	Joback Method
dvisc	0.0004682	Paxs	495.67	Joback Method
dvisc	0.0002920	Paxs	533.21	Joback Method
dvisc	0.0001938	Paxs	570.75	Joback Method
dvisc	0.0001353	Paxs	608.30	Joback Method
dvisc	0.0000985	Paxs	645.84	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C59748902&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C59748902&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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