

# 2-Amino-5-bromobenzoic acid

<b>Other names:</b>	5-Bromo-2-aminobenzoic acid 5-Bromoanthranilic acid Anthranilic acid, 5-bromo- Benzoic acid, 2-amino-5-bromo-
<b>Inchi:</b>	InChI=1S/C7H6BrNO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H,10,11)
<b>InchiKey:</b>	CUKXRHLWPSBCTI-UHFFFAOYSA-N
<b>Formula:</b>	C7H6BrNO2
<b>SMILES:</b>	Nc1ccc(Br)cc1C(=O)O
<b>Mol. weight [g/mol]:</b>	216.03
<b>CAS:</b>	5794-88-7

## Physical Properties

Property code	Value	Unit	Source
gf	-83.76	kJ/mol	Joback Method
hf	-178.91	kJ/mol	Joback Method
hfus	23.32	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-3.07		Aqueous Solubility Prediction Method
logp	1.730		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
pc	5845.00	kPa	Joback Method
tb	680.94	K	Joback Method
tc	912.27	K	Joback Method
tf	473.92	K	Joback Method
vc	0.435	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.54	J/molxK	680.94	Joback Method
cpg	271.55	J/molxK	719.50	Joback Method
cpg	278.02	J/molxK	758.05	Joback Method
cpg	284.00	J/molxK	796.61	Joback Method

cpg	289.52	J/mol×K	835.16	Joback Method
cpg	294.60	J/mol×K	873.72	Joback Method
cpg	299.27	J/mol×K	912.27	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=C5794887&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5794887&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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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>hvp:</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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