

# Benzonitrile, 2-bromo-

<b>Other names:</b>	1-Bromo-2-cyanobenzene 2-bromobenzonitrile 2-cyanobromobenzene Benzonitrile, o-bromo- o-bromobenzonitrile o-bromocyanobenzene
<b>Inchi:</b>	InChI=1S/C7H4BrN/c8-7-4-2-1-3-6(7)5-9/h1-4H
<b>InchiKey:</b>	AFMPMSCZPVNPEM-UHFFFAOYSA-N
<b>Formula:</b>	C7H4BrN
<b>SMILES:</b>	N#Cc1cccc1Br
<b>Mol. weight [g/mol]:</b>	182.02
<b>CAS:</b>	2042-37-7

## Physical Properties

Property code	Value	Unit	Source
gf	258.34	kJ/mol	Joback Method
hf	228.46	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.321		Crippen Method
mcvol	104.610	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	525.20	K	NIST Webbook
tc	812.58	K	Joback Method
tf	329.00	K	NIST Webbook
tf	327.10	K	Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on Iodobenzonitrile
vc	0.407	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.17	J/mol×K	559.46	Joback Method
cpg	195.99	J/mol×K	601.65	Joback Method
cpg	203.16	J/mol×K	643.83	Joback Method
cpg	209.74	J/mol×K	686.02	Joback Method
cpg	215.77	J/mol×K	728.21	Joback Method
cpg	221.29	J/mol×K	770.39	Joback Method
cpg	226.35	J/mol×K	812.58	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	525.20	K	101.00	NIST Webbook
tbrp	525.00 ± 1.00	K	101.00	NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Thermodynamic and aromaticity studies for the assessment of the hydrogen bond interactions on iodobenzonitrile:  
Halgam-Meyer and McGowan Method:

<https://www.doi.org/10.1016/j.jct.2013.06.003>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2042377&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure

<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/14-400-1/Benzonitrile-2-bromo.pdf>

Generated by Cheméo on 2024-04-19 19:01:13.75959421 +0000 UTC m=+15842522.680171531.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.