

# Benzonitrile, 2-amino-

<b>Other names:</b>	Anthranilonitrile o-Aminobenzonitrile o-Cyanoaniline Benzonitrile, o-amino- 2-Aminobenzonitrile 2-Cyano-1-aminobenzene 2-Cyanoaniline
<b>Inchi:</b>	InChI=1S/C7H6N2/c8-5-6-3-1-2-4-7(6)9/h1-4H,9H2
<b>InchiKey:</b>	HLCPWBZNUKCSBN-UHFFFAOYSA-N
<b>Formula:</b>	C7H6N2
<b>SMILES:</b>	N#Cc1ccccc1N
<b>Mol. weight [g/mol]:</b>	118.14
<b>CAS:</b>	1885-29-6

## Physical Properties

Property code	Value	Unit	Source
gf	310.47	kJ/mol	Joback Method
hf	235.92	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.140		Crippen Method
mvol	97.090	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	535.50 ± 0.50	K	NIST Webbook
tb	540.70	K	NIST Webbook
tc	812.67	K	Joback Method
tf	323.50 ± 0.50	K	NIST Webbook
vc	0.374	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.89	J/mol×K	565.83	Joback Method

cpg	214.76	J/mol×K	606.97	Joback Method
cpg	222.99	J/mol×K	648.11	Joback Method
cpg	230.59	J/mol×K	689.25	Joback Method
cpg	237.61	J/mol×K	730.39	Joback Method
cpg	244.08	J/mol×K	771.53	Joback Method
cpg	250.02	J/mol×K	812.67	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.00 ± 2.00	K	1.50	NIST Webbook

## 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=C1885296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1885296&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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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