

# Benzonitrile, 4-iodo-

<b>Other names:</b>	4-cyanoiodobenzene 4-cyanophenyl iodide 4-iodobenzonitrile Benzonitrile, p-iodo- p-cyanoiodobenzene p-cyanophenyl iodide p-iodobenzonitrile
<b>Inchi:</b>	InChI=1S/C7H4IN/c8-7-3-1-6(5-9)2-4-7/h1-4H
<b>InchiKey:</b>	XOKDXPVXJWTSRM-UHFFFAOYSA-N
<b>Formula:</b>	C7H4IN
<b>SMILES:</b>	N#Cc1ccc(I)cc1
<b>Mol. weight [g/mol]:</b>	229.02
<b>CAS:</b>	3058-39-7

## Physical Properties

Property code	Value	Unit	Source
gf	302.14	kJ/mol	Joback Method
hf	279.00	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	53.97	kJ/mol	Joback Method
ie	9.13	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.163		Crippen Method
mcvol	112.930	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	586.44	K	Joback Method
tc	857.62	K	Joback Method
tf	398.61	K	Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on Iodobenzonitrile
vc	0.433	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.95	J/molxK	586.44	Joback Method
cpg	202.63	J/molxK	631.64	Joback Method
cpg	209.62	J/molxK	676.83	Joback Method
cpg	215.97	J/molxK	722.03	Joback Method
cpg	221.74	J/molxK	767.23	Joback Method
cpg	226.99	J/molxK	812.42	Joback Method
cpg	231.79	J/molxK	857.62	Joback Method

## Sources

<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=C3058397&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3058397&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>Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on iodobenzonitrile:</b>	<a href="https://www.doi.org/10.1016/j.jct.2013.06.003">https://www.doi.org/10.1016/j.jct.2013.06.003</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>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</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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