

# 2-Chloro-4-nitrobenzotrile

<b>Inchi:</b>	InChI=1S/C7H3ClN2O2/c8-7-3-6(10(11)12)2-1-5(7)4-9/h1-3H
<b>InchiKey:</b>	ZIGQFRQZYVQQDR-UHFFFAOYSA-N
<b>Formula:</b>	C7H3ClN2O2
<b>SMILES:</b>	N#Cc1ccc([N+](=O)[O-])cc1Cl
<b>Mol. weight [g/mol]:</b>	182.56
<b>CAS:</b>	28163-00-0

## Physical Properties

Property code	Value	Unit	Source
gf	258.01	kJ/mol	Joback Method
hf	164.16	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	66.23	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.120		Crippen Method
mcvol	116.770	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	687.55	K	Joback Method
tc	954.98	K	Joback Method
tf	458.63	K	Joback Method
vc	0.476	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.20	J/mol×K	687.55	Joback Method
cpg	256.38	J/mol×K	732.12	Joback Method
cpg	262.90	J/mol×K	776.69	Joback Method
cpg	268.79	J/mol×K	821.27	Joback Method
cpg	274.08	J/mol×K	865.84	Joback Method
cpg	278.83	J/mol×K	910.41	Joback Method
cpg	283.06	J/mol×K	954.98	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=C28163000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28163000&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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