

# Benzeneacetonitrile, 3-chloro-

<b>Other names:</b>	Acetonitrile, (m-chlorophenyl)- (m-Chlorophenyl)acetonitrile m-Chlorobenzyl cyanide 3-(Chlorophenyl)acetonitrile 3-Chlorobenzyl cyanide
<b>Inchi:</b>	InChI=1S/C8H6ClN/c9-8-3-1-2-7(6-8)4-5-10/h1-3,6H,4H2
<b>InchiKey:</b>	GTIKLPYCSAMPNG-UHFFFAOYSA-N
<b>Formula:</b>	C8H6ClN
<b>SMILES:</b>	N#CCc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	151.59
<b>CAS:</b>	1529-41-5

## Physical Properties

Property code	Value	Unit	Source
gf	240.51	kJ/mol	Joback Method
hf	165.75	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
ie	9.48 ± 0.05	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.406		Crippen Method
mcvol	113.440	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	553.61	K	Joback Method
tc	791.13	K	Joback Method
tf	313.77	K	Joback Method
vc	0.451	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.76	J/mol×K	553.61	Joback Method
cpg	232.04	J/mol×K	593.20	Joback Method
cpg	240.67	J/mol×K	632.78	Joback Method

cpg	248.68	J/mol×K	672.37	Joback Method
cpg	256.09	J/mol×K	711.95	Joback Method
cpg	262.95	J/mol×K	751.54	Joback Method
cpg	269.27	J/mol×K	791.13	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	1.30	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=C1529415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1529415&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>ie:</b>	Ionization energy
<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
<b>vc:</b>	Critical Volume

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