

# 3-Chloro-4-methylbenzonitrile

<b>Other names:</b>	Benzonitrile, 3-chloro-4-methyl- 3-chloro-p-toluonitrile
<b>Inchi:</b>	InChI=1S/C8H6ClN/c1-6-2-3-7(5-10)4-8(6)9/h2-4H,1H3
<b>InchiKey:</b>	INEMHABDFCKBID-UHFFFAOYSA-N
<b>Formula:</b>	C8H6ClN
<b>SMILES:</b>	Cc1ccc(C#N)cc1Cl
<b>Mol. weight [g/mol]:</b>	151.59
<b>CAS:</b>	21423-81-4

## Physical Properties

Property code	Value	Unit	Source
gf	230.88	kJ/mol	Joback Method
hf	154.28	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.520		Crippen Method
mvol	113.440	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	558.59	K	Joback Method
tc	797.23	K	Joback Method
tf	326.29	K	Joback Method
vc	0.451	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.61	J/mol×K	558.59	Joback Method
cpg	230.58	J/mol×K	598.36	Joback Method
cpg	238.96	J/mol×K	638.14	Joback Method
cpg	246.78	J/mol×K	677.91	Joback Method
cpg	254.06	J/mol×K	717.68	Joback Method
cpg	260.81	J/mol×K	757.46	Joback Method
cpg	267.08	J/mol×K	797.23	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=C21423814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21423814&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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