

# 5-Chlorovaleronitrile

<b>Other names:</b>	5-Chloro-n-valeronitrile Pentanenitrile, 5-chloro- «delta»-Chlorovaleronitrile Valeronitrile, 5-chloro- 5-Chloropentanenitrile
<b>Inchi:</b>	InChI=1S/C5H8CIN/c6-4-2-1-3-5-7/h1-4H2
<b>InchiKey:</b>	JSAWFGSXRPCFSW-UHFFFAOYSA-N
<b>Formula:</b>	C5H8CIN
<b>SMILES:</b>	N#CCCCCI
<b>Mol. weight [g/mol]:</b>	117.58
<b>CAS:</b>	6280-87-1

## Physical Properties

Property code	Value	Unit	Source
gf	112.47	kJ/mol	Joback Method
hf	2.61	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.919		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	453.31	K	Joback Method
tc	650.81	K	Joback Method
tf	241.02	K	Joback Method
vc	0.391	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.73	J/mol×K	453.31	Joback Method
cpg	182.33	J/mol×K	486.23	Joback Method
cpg	189.58	J/mol×K	519.14	Joback Method
cpg	196.49	J/mol×K	552.06	Joback Method

cpg	203.06	J/mol×K	584.97	Joback Method
cpg	209.31	J/mol×K	617.89	Joback Method
cpg	215.26	J/mol×K	650.81	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=C6280871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6280871&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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