

# 2,5-Dichlorobenzonitrile

<b>Other names:</b>	Benzonitrile, 2,5-dichloro-
<b>Inchi:</b>	InChI=1S/C7H3Cl2N/c8-6-1-2-7(9)5(3-6)4-10/h1-3H
<b>InchiKey:</b>	LNGWRTKJZCBXGT-UHFFFAOYSA-N
<b>Formula:</b>	C7H3Cl2N
<b>SMILES:</b>	N#Cc1cc(Cl)ccc1Cl
<b>Mol. weight [g/mol]:</b>	172.01
<b>CAS:</b>	21663-61-6

## Physical Properties

Property code	Value	Unit	Source
gf	210.53	kJ/mol	Joback Method
hf	159.18	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	54.02	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.865		Crippen Method
mcvol	111.590	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	573.14	K	Joback Method
tc	820.89	K	Joback Method
tf	344.94	K	Joback Method
vc	0.444	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.82	J/mol×K	573.14	Joback Method
cpg	205.80	J/mol×K	614.43	Joback Method
cpg	212.24	J/mol×K	655.72	Joback Method
cpg	218.19	J/mol×K	697.01	Joback Method
cpg	223.66	J/mol×K	738.31	Joback Method
cpg	228.67	J/mol×K	779.60	Joback Method
cpg	233.27	J/mol×K	820.89	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21663616&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21663616&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>hvp:</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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