

# 2,2-Dichlorocyclopropylacetonitrile

<b>Inchi:</b>	InChI=1S/C5H5Cl2N/c6-5(7)3-4(5)1-2-8/h4H,1,3H2
<b>InchiKey:</b>	METYSMJJRFRDPP-UHFFFAOYSA-N
<b>Formula:</b>	C5H5Cl2N
<b>SMILES:</b>	N#CCC1CC1(Cl)Cl
<b>Mol. weight [g/mol]:</b>	150.01
<b>CAS:</b>	5365-25-3

## Physical Properties

Property code	Value	Unit	Source
gf	148.09	kJ/mol	Joback Method
hf	54.57	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.094		Crippen Method
mvol	96.310	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	493.05	K	Joback Method
tc	722.51	K	Joback Method
tf	308.54	K	Joback Method
vc	0.394	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.89	J/mol×K	493.05	Joback Method
cpg	189.65	J/mol×K	531.29	Joback Method
cpg	196.60	J/mol×K	569.54	Joback Method
cpg	202.91	J/mol×K	607.78	Joback Method
cpg	208.71	J/mol×K	646.02	Joback Method
cpg	214.15	J/mol×K	684.27	Joback Method
cpg	219.37	J/mol×K	722.51	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5365253&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5365253&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>mccvol:</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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