

# Propanedinitrile, methylene-

Other names:	Malononitrile, methylene-Vinylidene cyanide 1,1-Dicyanoethylene 1,1-Ethenedicarbonitrile
Inchi:	InChI=1S/C4H2N2/c1-4(2-5)3-6/h1H2
InchiKey:	FCYVWWWTHPPJII-UHFFFAOYSA-N
Formula:	C4H2N2
SMILES:	C=C(C#N)C#N
Mol. weight [g/mol]:	78.07
CAS:	922-64-5

## Physical Properties

Property code	Value	Unit	Source
gf	328.45	kJ/mol	Joback Method
hf	319.51	kJ/mol	Joback Method
hfus	6.54	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
ie	11.38 ± 0.05	eV	NIST Webbook
log10ws	-1.08		Crippen Method
logp	0.590		Crippen Method
mcvol	65.680	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	491.64	K	Joback Method
tc	715.64	K	Joback Method
tf	249.10	K	Joback Method
vc	0.293	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.43	J/molxK	491.64	Joback Method
cpg	116.41	J/molxK	528.97	Joback Method
cpg	120.15	J/molxK	566.31	Joback Method
cpg	123.65	J/molxK	603.64	Joback Method

cpg	126.93	J/mol×K	640.98	Joback Method
cpg	130.00	J/mol×K	678.31	Joback Method
cpg	132.88	J/mol×K	715.64	Joback Method

## Sources

<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=C922645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C922645&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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