

# 1,4-Benzenediacetonitrile

<b>Other names:</b>	p-Benzenediacetonitrile p-(Cyanomethyl)benzyl cyanide p-Bis(cyanomethyl)benzene p-Phenylenediacetonitrile p-Xylylene dicyanide 1,4-Bis(cyanomethyl)benzene 1,4-Phenylenediacetonitrile
<b>Inchi:</b>	InChI=1S/C10H8N2/c11-7-5-9-1-2-10(4-3-9)6-8-12/h1-4H,5-6H2
<b>InchiKey:</b>	FUQCKESKNZBNOG-UHFFFAOYSA-N
<b>Formula:</b>	C10H8N2
<b>SMILES:</b>	N#CCc1ccc(CC#N)cc1
<b>Mol. weight [g/mol]:</b>	156.18
<b>CAS:</b>	622-75-3

## Physical Properties

Property code	Value	Unit	Source
gf	402.46	kJ/mol	Joback Method
hf	305.09	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	61.75	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.819		Crippen Method
mvol	130.760	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	664.02	K	Joback Method
tc	902.09	K	Joback Method
tf	371.38	K	Joback Method
vc	0.539	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.87	J/mol×K	664.02	Joback Method
cpg	314.46	J/mol×K	703.70	Joback Method

cpg	323.36	J/mol×K	743.38	Joback Method
cpg	331.60	J/mol×K	783.05	Joback Method
cpg	339.22	J/mol×K	822.73	Joback Method
cpg	346.26	J/mol×K	862.41	Joback Method
cpg	352.75	J/mol×K	902.09	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C622753&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C622753&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.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>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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