

# Benzoic acid, 4-cyano-

<b>Other names:</b>	4-Carboxybenzonitrile 4-cyanobenzoic acid Benzoic acid, p-cyano- Terephthalic mononitrile p-Carboxybenzonitrile p-cyanobenzoic acid
<b>Inchi:</b>	InChI=1S/C8H5NO2/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4H,(H,10,11)
<b>InchiKey:</b>	ADCUEPOHPCPMCE-UHFFFAOYSA-N
<b>Formula:</b>	C8H5NO2
<b>SMILES:</b>	N#Cc1ccc(C(=O)O)cc1
<b>Mol. weight [g/mol]:</b>	147.13
<b>CAS:</b>	619-65-8

## Physical Properties

Property code	Value	Unit	Source
gf	-13.30	kJ/mol	Joback Method
hf	-83.32	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hsub	112.80 ± 0.40	kJ/mol	NIST Webbook
hvap	70.24	kJ/mol	Joback Method
ie	10.30 ± 0.20	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.256		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	662.23	K	Joback Method
tc	883.54	K	Joback Method
tf	394.60	K	Joback Method
vc	0.426	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	247.34	J/mol×K	662.23	Joback Method
cpg	254.39	J/mol×K	699.12	Joback Method
cpg	260.92	J/mol×K	736.00	Joback Method
cpg	266.96	J/mol×K	772.89	Joback Method
cpg	272.52	J/mol×K	809.77	Joback Method
cpg	277.64	J/mol×K	846.66	Joback Method
cpg	282.34	J/mol×K	883.54	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=C619658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C619658&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>Solubility of 3,5-Dimethoxybenzoic Acid, 4-Cyanobenzoic Acid, 4-Acetoxybenzoic Acid, 3,5-Diaminobenzoic Acid, and 2,4-Dichlorobenzoic Acid in Ethanol:</b>	<a href="https://www.doi.org/10.1021/je900190n">https://www.doi.org/10.1021/je900190n</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>hsub:</b>	Enthalpy of sublimation 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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