

# Benzonitrile, 4-fluoro-

<b>Other names:</b>	Benzonitrile, p-fluoro- p-Cyanofluorobenzene p-Fluorobenzonitrile 4-Fluorobenzonitrile
<b>Inchi:</b>	InChI=1S/C7H4FN/c8-7-3-1-6(5-9)2-4-7/h1-4H
<b>InchiKey:</b>	AEKVBBNGWBBYLL-UHFFFAOYSA-N
<b>Formula:</b>	C7H4FN
<b>SMILES:</b>	N#Cc1ccc(F)cc1
<b>Mol. weight [g/mol]:</b>	121.11
<b>CAS:</b>	1194-02-1

## Physical Properties

Property code	Value	Unit	Source
gf	49.21	kJ/mol	Joback Method
hf	6.02	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	43.78	kJ/mol	Joback Method
ie	9.74	eV	NIST Webbook
ie	9.99 ± 0.05	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	1.697		Crippen Method
mcvol	88.880	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	461.00	K	NIST Webbook
tc	717.07	K	Joback Method
tf	273.17	K	Joback Method
vc	0.363	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.19	J/mol×K	492.57	Joback Method
cpg	177.42	J/mol×K	529.99	Joback Method
cpg	185.12	J/mol×K	567.40	Joback Method

cpg	192.30	J/mol×K	604.82	Joback Method
cpg	198.98	J/mol×K	642.24	Joback Method
cpg	205.20	J/mol×K	679.66	Joback Method
cpg	210.97	J/mol×K	717.07	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	461.20	K	100.00	NIST Webbook

## 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=C1194021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1194021&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>

## 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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