

# 2-Fluoro-5-nitrobenzonitrile

<b>Inchi:</b>	InChI=1S/C7H3FN2O2/c8-7-2-1-6(10(11)12)3-5(7)4-9/h1-3H
<b>InchiKey:</b>	YLACBMHBZVYOAP-UHFFFAOYSA-N
<b>Formula:</b>	C7H3FN2O2
<b>SMILES:</b>	N#Cc1cc([N+](=O)[O-])ccc1F
<b>Mol. weight [g/mol]:</b>	166.11
<b>CAS:</b>	17417-09-3

## Physical Properties

Property code	Value	Unit	Source
gf	75.13	kJ/mol	Joback Method
hf	-16.21	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.606		Crippen Method
mcvol	106.300	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	649.39	K	Joback Method
tc	901.51	K	Joback Method
tf	429.30	K	Joback Method
vc	0.446	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.70	J/molxK	649.39	Joback Method
cpg	247.29	J/molxK	691.41	Joback Method
cpg	254.26	J/molxK	733.43	Joback Method
cpg	260.62	J/molxK	775.45	Joback Method
cpg	266.41	J/molxK	817.47	Joback Method
cpg	271.66	J/molxK	859.49	Joback Method
cpg	276.39	J/molxK	901.51	Joback Method

# Sources

<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>
<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=C17417093&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17417093&amp;Units=SI</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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