

# Benzeneacetonitrile, 3-nitro-

<b>Other names:</b>	Acetonitrile, (m-nitrophenyl)- m-Nitro-phenylacetonitrile m-Nitrobenzyl cyanide 3-nitrophenylacetonitrile
<b>Inchi:</b>	InChI=1S/C8H6N2O2/c9-5-4-7-2-1-3-8(6-7)10(11)12/h1-3,6H,4H2
<b>InchiKey:</b>	WAVKEPUFQMUGBP-UHFFFAOYSA-N
<b>Formula:</b>	C8H6N2O2
<b>SMILES:</b>	<chem>N#CCc1cccc([N+](=O)[O-])c1</chem>
<b>Mol. weight [g/mol]:</b>	162.15
<b>CAS:</b>	621-50-1

## Physical Properties

Property code	Value	Unit	Source
gf	287.99	kJ/mol	Joback Method
hf	170.73	kJ/mol	Joback Method
hfus	23.00	kJ/mol	Joback Method
hvap	63.41	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	1.661		Crippen Method
mcvol	118.620	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	668.02	K	Joback Method
tc	926.02	K	Joback Method
tf	427.46	K	Joback Method
vc	0.483	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.60	J/molxK	668.02	Joback Method
cpg	288.90	J/molxK	711.02	Joback Method
cpg	297.41	J/molxK	754.02	Joback Method
cpg	305.17	J/molxK	797.02	Joback Method
cpg	312.24	J/molxK	840.02	Joback Method

cpg	318.66	J/mol×K	883.02	Joback Method
cpg	324.47	J/mol×K	926.02	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C621501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C621501&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>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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