

# N-methyl-n-nitro amino acetonitrile

<b>Inchi:</b>	InChI=1S/C3H5N3O2/c1-5(3-2-4)6(7)8/h3H2,1H3
<b>InchiKey:</b>	MOXABXZIUXZMCH-UHFFFAOYSA-N
<b>Formula:</b>	C3H5N3O2
<b>SMILES:</b>	CN(CC#N)[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	115.09
<b>CAS:</b>	20661-61-4

## Physical Properties

Property code	Value	Unit	Source
gf	253.89	kJ/mol	Joback Method
hf	116.40	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	-0.367		Crippen Method
mcvol	81.910	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	534.40	K	Joback Method
tc	761.60	K	Joback Method
tf	364.64	K	Joback Method
vc	0.330	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.78	J/molxK	534.40	Joback Method
cpg	183.78	J/molxK	572.27	Joback Method
cpg	190.29	J/molxK	610.13	Joback Method
cpg	196.34	J/molxK	648.00	Joback Method
cpg	201.95	J/molxK	685.87	Joback Method
cpg	207.14	J/molxK	723.73	Joback Method
cpg	211.95	J/molxK	761.60	Joback Method

# Sources

<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=C20661614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20661614&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>

# 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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