

# Benzamide, 2-chloro-n-(cyanomethyl)-n-ethyl-4-nitro-

Inchi:	InChI=1S/C11H10ClN3O3/c1-2-14(6-5-13)11(16)9-4-3-8(15(17)18)7-10(9)12/h3-4,7H,2,6
InchiKey:	WENFSKFNPFJJPQ-UHFFFAOYSA-N
Formula:	C11H10ClN3O3
SMILES:	CCN(CC#N)C(=O)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	267.67
CAS:	22977-88-4

## Physical Properties

Property code	Value	Unit	Source
gf	273.55	kJ/mol	Joback Method
hf	36.55	kJ/mol	Joback Method
hfus	39.19	kJ/mol	Joback Method
hvap	83.92	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.234		Crippen Method
mcvol	184.680	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
tb	845.38	K	Joback Method
tc	1090.78	K	Joback Method
tf	586.11	K	Joback Method
vc	0.725	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.36	J/molxK	845.38	Joback Method
cpg	499.36	J/molxK	886.28	Joback Method
cpg	507.53	J/molxK	927.18	Joback Method
cpg	514.95	J/molxK	968.08	Joback Method
cpg	521.67	J/molxK	1008.98	Joback Method
cpg	527.75	J/molxK	1049.88	Joback Method
cpg	533.26	J/molxK	1090.78	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22977884&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22977884&amp;Units=SI</a>
<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>

# 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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