

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

Inchi:	InChI=1S/C12H12ClN3O3/c1-2-6-15(7-5-14)12(17)10-4-3-9(16(18)19)8-11(10)13/h3-4,8
InchiKey:	YPTXIFWZSOODGM-UHFFFAOYSA-N
Formula:	C12H12ClN3O3
SMILES:	CCCN(CC#N)C(=O)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	281.69
CAS:	22977-93-1

## Physical Properties

Property code	Value	Unit	Source
gf	281.97	kJ/mol	Joback Method
hf	15.91	kJ/mol	Joback Method
hfus	41.78	kJ/mol	Joback Method
hvap	86.15	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.624		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	868.26	K	Joback Method
tc	1109.74	K	Joback Method
tf	597.38	K	Joback Method
vc	0.780	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.85	J/molxK	868.26	Joback Method
cpg	553.32	J/molxK	908.51	Joback Method
cpg	561.95	J/molxK	948.75	Joback Method
cpg	569.82	J/molxK	989.00	Joback Method
cpg	576.98	J/molxK	1029.25	Joback Method
cpg	583.49	J/molxK	1069.50	Joback Method
cpg	589.41	J/molxK	1109.74	Joback Method

# 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=C22977931&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22977931&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>

# 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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