

# Acetanilide, n-beta-cyanoethyl-

<b>Inchi:</b>	InChI=1S/C11H12N2O/c1-10(14)13(9-5-8-12)11-6-3-2-4-7-11/h2-4,6-7H,5,9H2,1H3
<b>InchiKey:</b>	XPTMZUGVSAGQME-UHFFFAOYSA-N
<b>Formula:</b>	C11H12N2O
<b>SMILES:</b>	CC(=O)N(CCC#N)c1ccccc1
<b>Mol. weight [g/mol]:</b>	188.23
<b>CAS:</b>	104086-54-6

## Physical Properties

Property code	Value	Unit	Source
gf	269.19	kJ/mol	Joback Method
hf	85.99	kJ/mol	Joback Method
hfus	24.41	kJ/mol	Joback Method
hvap	61.62	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.953		Crippen Method
mcvol	155.020	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
tb	646.15	K	Joback Method
tc	869.10	K	Joback Method
tf	387.54	K	Joback Method
vc	0.594	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.14	J/molxK	646.15	Joback Method
cpg	397.52	J/molxK	683.31	Joback Method
cpg	409.01	J/molxK	720.47	Joback Method
cpg	419.65	J/molxK	757.62	Joback Method
cpg	429.50	J/molxK	794.78	Joback Method
cpg	438.59	J/molxK	831.94	Joback Method
cpg	447.00	J/molxK	869.10	Joback Method

# Sources

<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=C104086546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C104086546&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>

# 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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