

# N-Acetyl-L-tyrosinamide

<b>Other names:</b>	N-Acetyl-L-tyrosine amide N-«alpha»-Acetyl-L-tyrosinamide Benzenepropanamide, «alpha»-(acetylamino)-4-hydroxy-, (S)-
<b>Inchi:</b>	InChI=1S/C11H14N2O3/c1-7(14)13-10(11(12)16)6-8-2-4-9(15)5-3-8/h2-5,10,15H,6H2,1H
<b>InchiKey:</b>	RJNKBEQRBIJDNM-SNVBAGLBSA-N
<b>Formula:</b>	C11H14N2O3
<b>SMILES:</b>	CC(=O)NC(Cc1ccc(O)cc1)C(N)=O
<b>Mol. weight [g/mol]:</b>	222.24
<b>CAS:</b>	1948-71-6

## Physical Properties

Property code	Value	Unit	Source
gf	-104.91	kJ/mol	Joback Method
hf	-354.33	kJ/mol	Joback Method
hfus	34.04	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	-0.075		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	788.38	K	Joback Method
tc	1024.77	K	Joback Method
tf	572.65	K	Joback Method
vc	0.580	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.31	J/molxK	788.38	Joback Method
cpg	501.22	J/molxK	827.78	Joback Method
cpg	511.43	J/molxK	867.18	Joback Method
cpg	521.06	J/molxK	906.57	Joback Method
cpg	530.21	J/molxK	945.97	Joback Method
cpg	538.98	J/molxK	985.37	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=C1948716&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1948716&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>

## 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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