

# (4-Aminobenzoyl)acetonitrile

<b>Other names:</b>	Benzenepropanenitrile, 4-amino-«beta»-oxo-Propionitrile, 3-(4-aminophenyl)-3-oxo-(p-Aminobenzoyl)acetonitrile
<b>Inchi:</b>	InChI=1S/C9H8N2O/c10-6-5-9(12)7-1-3-8(11)4-2-7/h1-4H,5,11H2
<b>InchiKey:</b>	BEWGVKVVWWKCFHO-UHFFFAOYSA-N
<b>Formula:</b>	C9H8N2O
<b>SMILES:</b>	N#CCC(=O)c1ccc(N)cc1
<b>Mol. weight [g/mol]:</b>	160.17
<b>CAS:</b>	59443-94-6

## Physical Properties

Property code	Value	Unit	Source
gf	198.39	kJ/mol	Joback Method
hf	82.06	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	66.43	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.365		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	665.46	K	Joback Method
tc	908.44	K	Joback Method
tf	428.31	K	Joback Method
vc	0.492	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.07	J/molxK	665.46	Joback Method
cpg	313.71	J/molxK	705.96	Joback Method
cpg	322.60	J/molxK	746.45	Joback Method
cpg	330.78	J/molxK	786.95	Joback Method
cpg	338.29	J/molxK	827.45	Joback Method
cpg	345.15	J/molxK	867.94	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=C59443946&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C59443946&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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