

# beta-aminobutyric acid

<b>Inchi:</b>	InChI=1S/C4H9NO2/c1-3(5)2-4(6)7/h3H,2,5H2,1H3,(H,6,7)
<b>InchiKey:</b>	OQEBBZSWEGYTPG-UHFFFAOYSA-N
<b>Formula:</b>	C4H9NO2
<b>SMILES:</b>	CC(N)CC(=O)O
<b>Mol. weight [g/mol]:</b>	103.12

## Physical Properties

Property code	Value	Unit	Source
gf	-218.93	kJ/mol	Joback Method
hf	-362.19	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	1.08		Aqueous Solubility Prediction Method
logp	-0.192		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	509.06	K	Joback Method
tc	698.51	K	Joback Method
tf	313.85	K	Joback Method
vc	0.307	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.62	J/mol×K	509.06	Joback Method
cpg	197.96	J/mol×K	540.64	Joback Method
cpg	204.95	J/mol×K	572.21	Joback Method
cpg	211.60	J/mol×K	603.79	Joback Method
cpg	217.92	J/mol×K	635.36	Joback Method
cpg	223.92	J/mol×K	666.94	Joback Method
cpg	229.60	J/mol×K	698.51	Joback Method

# Sources

<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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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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