

# L-2-Aminobutyric acid, N-methyl-, methyl ester

<b>Other names:</b>	Methyl (2R)-2-(methylamino)butanoate
<b>Inchi:</b>	InChI=1S/C6H13NO2/c1-4-5(7-2)6(8)9-3/h5,7H,4H2,1-3H3
<b>InchiKey:</b>	INBBIXRVEUBDRU-UHFFFAOYSA-N
<b>Formula:</b>	C6H13NO2
<b>SMILES:</b>	CCC(NC)C(=O)OC
<b>Mol. weight [g/mol]:</b>	131.17

## Physical Properties

Property code	Value	Unit	Source
gf	-147.33	kJ/mol	Joback Method
hf	-363.78	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.157		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	900.40		NIST Webbook
rinpol	900.40		NIST Webbook
tb	462.70	K	Joback Method
tc	648.02	K	Joback Method
tf	267.20	K	Joback Method
vc	0.424	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.24	J/mol×K	462.70	Joback Method
cpg	252.18	J/mol×K	493.59	Joback Method
cpg	262.71	J/mol×K	524.47	Joback Method
cpg	272.83	J/mol×K	555.36	Joback Method
cpg	282.54	J/mol×K	586.25	Joback Method
cpg	291.85	J/mol×K	617.13	Joback Method
cpg	300.75	J/mol×K	648.02	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U332987&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U332987&amp;Units=SI</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>rinpola:</b>	Non-polar retention indices
<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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