

# «beta»-Alanine, N-isobutyryl-, ethyl ester

<b>Inchi:</b>	InChI=1S/C9H17NO3/c1-4-13-8(11)5-6-10-9(12)7(2)3/h7H,4-6H2,1-3H3,(H,10,12)
<b>InchiKey:</b>	PFTYOYXLRHLHBCZ-UHFFFAOYSA-N
<b>Formula:</b>	C9H17NO3
<b>SMILES:</b>	CCOC(=O)CCNC(=O)C(C)C
<b>Mol. weight [g/mol]:</b>	187.24

## Physical Properties

Property code	Value	Unit	Source
gf	-250.99	kJ/mol	Joback Method
hf	-538.28	kJ/mol	Joback Method
hfus	25.03	kJ/mol	Joback Method
hvap	57.58	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.712		Crippen Method
mcvol	156.660	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinsol	1406.00		NIST Webbook
tb	585.21	K	Joback Method
tc	773.19	K	Joback Method
tf	350.94	K	Joback Method
vc	0.599	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.11	J/mol×K	585.21	Joback Method
cpg	406.08	J/mol×K	616.54	Joback Method
cpg	418.44	J/mol×K	647.87	Joback Method
cpg	430.20	J/mol×K	679.20	Joback Method
cpg	441.37	J/mol×K	710.53	Joback Method
cpg	451.95	J/mol×K	741.86	Joback Method
cpg	461.96	J/mol×K	773.19	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=U321661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321661&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.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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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

Latest version available from:

<https://www.chemeo.com/cid/41-493-9/beta-Alanine-N-isobutyryl-ethyl-ester.pdf>

Generated by Cheméo on 2024-05-02 22:38:42.266499619 +0000 UTC m=+16978771.187076952.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.