

# L-Isoleucine, ethyl ester

<b>Other names:</b>	Isoleucine, ethyl ester, L-ethyl L-isoleucinate
<b>Inchi:</b>	InChI=1S/C8H17NO2/c1-4-6(3)7(9)8(10)11-5-2/h6-7H,4-5,9H2,1-3H3/t6-,7-/m1/s1
<b>InchiKey:</b>	ICPWNTVICOHCML-RNFRBKRXSA-N
<b>Formula:</b>	C8H17NO2
<b>SMILES:</b>	CCOC(=O)C(N)C(C)CC
<b>Mol. weight [g/mol]:</b>	159.23
<b>CAS:</b>	921-74-4

## Physical Properties

Property code	Value	Unit	Source
gf	-155.87	kJ/mol	Joback Method
hf	-430.02	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.923		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpola	1114.00		NIST Webbook
tb	530.38	K	Joback Method
tc	724.15	K	Joback Method
tf	305.34	K	Joback Method
vc	0.524	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.70	J/mol×K	530.38	Joback Method
cpg	351.98	J/mol×K	562.68	Joback Method
cpg	364.67	J/mol×K	594.97	Joback Method
cpg	376.78	J/mol×K	627.27	Joback Method
cpg	388.32	J/mol×K	659.56	Joback Method
cpg	399.29	J/mol×K	691.86	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C921744&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C921744&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>
<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>

## 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>rinpol:</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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