

# Leu, isopropyl ester

<b>Inchi:</b>	InChI=1S/C9H19NO2/c1-6(2)5-8(10)9(11)12-7(3)4/h6-8H,5,10H2,1-4H3
<b>InchiKey:</b>	KDESEECZHLTGMH-UHFFFAOYSA-N
<b>Formula:</b>	C9H19NO2
<b>SMILES:</b>	CC(C)CC(N)C(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	173.25

## Physical Properties

Property code	Value	Unit	Source
gf	-149.89	kJ/mol	Joback Method
hf	-455.94	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.311		Crippen Method
mcvol	155.090	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1217.00		NIST Webbook
tb	552.82	K	Joback Method
tc	748.04	K	Joback Method
tf	301.61	K	Joback Method
vc	0.575	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.51	J/molxK	552.82	Joback Method
cpg	399.99	J/molxK	585.36	Joback Method
cpg	413.79	J/molxK	617.89	Joback Method
cpg	426.93	J/molxK	650.43	Joback Method
cpg	439.42	J/molxK	682.97	Joback Method
cpg	451.27	J/molxK	715.51	Joback Method

## Sources

<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=R535834&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R535834&amp;Units=SI</a>
<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>

## 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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