

# L-Leucine, N-allyloxycarbonyl-N-methyl-, dodecyl ester

<b>Inchi:</b>	InChI=1S/C23H43NO4/c1-6-8-9-10-11-12-13-14-15-16-18-27-22(25)21(19-20(3)4)24(5)2
<b>InchiKey:</b>	VIFJAVGJSPVRCE-UHFFFAOYSA-N
<b>Formula:</b>	C23H43NO4
<b>SMILES:</b>	C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	397.59

## Physical Properties

Property code	Value	Unit	Source
gf	-131.32	kJ/mol	Joback Method
hf	-825.25	kJ/mol	Joback Method
hfus	55.60	kJ/mol	Joback Method
hvap	85.70	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.120		Crippen Method
mvol	355.490	ml/mol	McGowan Method
pc	930.64	kPa	Joback Method
rinpol	2497.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	886.46	K	Joback Method
tc	1085.29	K	Joback Method
tf	494.00	K	Joback Method
vc	1.359	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.10	J/molxK	886.46	Joback Method
cpg	1190.29	J/molxK	919.60	Joback Method
cpg	1208.19	J/molxK	952.74	Joback Method
cpg	1224.83	J/molxK	985.87	Joback Method
cpg	1240.26	J/molxK	1019.01	Joback Method
cpg	1254.52	J/molxK	1052.15	Joback Method
cpg	1267.65	J/molxK	1085.29	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=U321905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321905&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>hvp:</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>rinp:</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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