

# L-Leucine, N-methyl-N-(but-3-yn-1-yloxy carbonyl)-, pentadecyl ester

InChI: InChI=1S/C27H49NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-22-31-26(29)25(23-24)3  
InChIKey: VDFWGGJUZAMXMLI-RUZDIDTESA-N

Formula: C27H49NO4

SMILES: C#CCCCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 451.68

## Physical Properties

Property code	Value	Unit	Source
gf	37.59	kJ/mol	Joback Method
hf	-741.34	kJ/mol	Joback Method
hfus	70.21	kJ/mol	Joback Method
hvap	95.13	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.127		Crippen Method
mvol	407.550	ml/mol	McGowan Method
pc	790.82	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	971.42	K	Joback Method
tc	1194.42	K	Joback Method
tf	587.81	K	Joback Method
vc	1.563	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1392.86	J/molxK	971.42	Joback Method
cpg	1413.33	J/molxK	1008.59	Joback Method
cpg	1432.19	J/molxK	1045.75	Joback Method
cpg	1449.51	J/molxK	1082.92	Joback Method
cpg	1465.37	J/molxK	1120.08	Joback Method
cpg	1479.84	J/molxK	1157.25	Joback Method
cpg	1492.99	J/molxK	1194.42	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=U392382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392382&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.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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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