

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

InChI: InChI=1S/C29H53NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-24-33-28(31)27  
InChIKey: BZMLXZJXMKGGAQ-HHHXNRCGSA-N

Formula: C29H53NO4

SMILES: C#CCCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 479.74

## Physical Properties

Property code	Value	Unit	Source
gf	54.43	kJ/mol	Joback Method
hf	-782.62	kJ/mol	Joback Method
hfus	75.39	kJ/mol	Joback Method
hvap	99.59	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	7.907		Crippen Method
mvol	435.730	ml/mol	McGowan Method
pc	711.87	kPa	Joback Method
rinpol	3026.00		NIST Webbook
rinpol	3026.00		NIST Webbook
tb	1017.18	K	Joback Method
tc	1259.83	K	Joback Method
tf	610.35	K	Joback Method
vc	1.675	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.76	J/molxK	1017.18	Joback Method
cpg	1543.47	J/molxK	1057.62	Joback Method
cpg	1563.29	J/molxK	1098.06	Joback Method
cpg	1581.31	J/molxK	1138.50	Joback Method
cpg	1597.63	J/molxK	1178.94	Joback Method
cpg	1612.37	J/molxK	1219.38	Joback Method
cpg	1625.61	J/molxK	1259.83	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=U392384&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392384&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>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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