

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

InChI: InChI=1S/C30H55NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-34-29(32)  
InChIKey: JKGBFCJMPUNNNN-MUUNZHRXSA-N

Formula: C30H55NO4

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

Mol. weight [g/mol]: 493.76

## Physical Properties

Property code	Value	Unit	Source
gf	62.85	kJ/mol	Joback Method
hf	-803.26	kJ/mol	Joback Method
hfus	77.98	kJ/mol	Joback Method
hvap	101.81	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	8.297		Crippen Method
mvol	449.820	ml/mol	McGowan Method
pc	676.76	kPa	Joback Method
rinpol	3128.00		NIST Webbook
rinpol	3128.00		NIST Webbook
tb	1040.06	K	Joback Method
tc	1294.62	K	Joback Method
tf	621.62	K	Joback Method
vc	1.732	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1586.72	J/molxK	1040.06	Joback Method
cpg	1609.15	J/molxK	1082.49	Joback Method
cpg	1629.50	J/molxK	1124.91	Joback Method
cpg	1647.90	J/molxK	1167.34	Joback Method
cpg	1664.47	J/molxK	1209.76	Joback Method
cpg	1679.34	J/molxK	1252.19	Joback Method
cpg	1692.62	J/molxK	1294.62	Joback Method

# Sources

<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>
<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=U392385&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392385&amp;Units=SI</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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