

# L-Leucine, N-methyl-N-(but-3-yn-1-yloxycarbonyl)-, hexadecyl ester

InChI: InChI=1S/C28H51NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-23-32-27(30)26(24)25  
InChIKey: XBTWLRHMLVTJPO-AREMUKBSSA-N  
Formula: C28H51NO4  
SMILES: C#CCCCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCCCCCCCCCC  
Mol. weight [g/mol]: 465.71

## Physical Properties

Property code	Value	Unit	Source
gf	46.01	kJ/mol	Joback Method
hf	-761.98	kJ/mol	Joback Method
hfus	72.80	kJ/mol	Joback Method
hvap	97.36	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	7.517		Crippen Method
mcvol	421.640	ml/mol	McGowan Method
pc	749.79	kPa	Joback Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
tb	994.30	K	Joback Method
tc	1226.46	K	Joback Method
tf	599.08	K	Joback Method
vc	1.619	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.12	J/molxK	994.30	Joback Method
cpg	1478.19	J/molxK	1032.99	Joback Method
cpg	1497.51	J/molxK	1071.69	Joback Method
cpg	1515.17	J/molxK	1110.38	Joback Method
cpg	1531.25	J/molxK	1149.07	Joback Method
cpg	1545.86	J/molxK	1187.77	Joback Method
cpg	1559.06	J/molxK	1226.46	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=U392383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392383&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>

## 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>rlnpol:</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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