

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

Inchi:  
ester

InChI=1S/C16H27NO4/c1-6-8-10-20-15(18)14(12-13(3)4)17(5)16(19)21-11-9-7-2/h2,13-

InchiKey:

OYYVPTHZSQQLI-CQSZACIVSA-N

Formula:

C16H27NO4

SMILES:

C#CCCOC(=O)N(C)C(CC(C)C)C(=O)OCCCC

Mol. weight [g/mol]:

297.39

## Physical Properties

Property code	Value	Unit	Source
gf	-55.03	kJ/mol	Joback Method
hf	-514.30	kJ/mol	Joback Method
hfus	41.72	kJ/mol	Joback Method
hvap	70.65	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.836		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	719.74	K	Joback Method
tc	905.68	K	Joback Method
tf	463.84	K	Joback Method
vc	0.948	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.30	J/mol×K	719.74	Joback Method
cpg	741.52	J/mol×K	750.73	Joback Method
cpg	756.85	J/mol×K	781.72	Joback Method
cpg	771.30	J/mol×K	812.71	Joback Method
cpg	784.91	J/mol×K	843.70	Joback Method
cpg	797.68	J/mol×K	874.69	Joback Method
cpg	809.65	J/mol×K	905.68	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392374&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392374&amp;Units=SI</a>
<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>

# 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>hvpap:</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>rinppl:</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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