

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

InChI: InChI=1S/C16H23NO4/c1-6-8-10-20-15(18)14(12-13(3)4)17(5)16(19)21-11-9-7-2/h1-2,11-12,14-15,17-18,20-21/t16,18,20,21  
InChIKey: MXKLLPCZYUWVQOX-CQSZACIVSA-N

Formula: C16H23NO4

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

Mol. weight [g/mol]: 293.36

## Physical Properties

Property code	Value	Unit	Source
gf	168.04	kJ/mol	Joback Method
hf	-222.40	kJ/mol	Joback Method
hfus	44.69	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.059		Crippen Method
mcvol	243.960	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1814.00		NIST Webbook
rinpol	1814.00		NIST Webbook
tb	709.86	K	Joback Method
tc	903.73	K	Joback Method
tf	510.81	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.68	J/molxK	709.86	Joback Method
cpg	690.96	J/molxK	742.17	Joback Method
cpg	705.37	J/molxK	774.48	Joback Method
cpg	718.92	J/molxK	806.80	Joback Method
cpg	731.65	J/molxK	839.11	Joback Method
cpg	743.57	J/molxK	871.42	Joback Method
cpg	754.71	J/molxK	903.73	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.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>
<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=U392386&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392386&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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