

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

Inchi:  
ester

InChI=1S/C20H35NO4/c1-6-8-10-11-12-13-15-24-19(22)18(16-17(3)4)21(5)20(23)25-14

InchiKey:

NYZLDZIIIGCQPKA-GOSISDBHSA-N

Formula:

C20H35NO4

SMILES:

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

Mol. weight [g/mol]:

353.50

## Physical Properties

Property code	Value	Unit	Source
gf	-21.35	kJ/mol	Joback Method
hf	-596.86	kJ/mol	Joback Method
hfus	52.08	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.397		Crippen Method
mvol	308.920	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	811.26	K	Joback Method
tc	999.75	K	Joback Method
tf	508.92	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.49	J/molxK	811.26	Joback Method
cpg	975.02	J/molxK	842.68	Joback Method
cpg	991.50	J/molxK	874.09	Joback Method
cpg	1006.96	J/molxK	905.51	Joback Method
cpg	1021.43	J/molxK	936.92	Joback Method
cpg	1034.94	J/molxK	968.34	Joback Method
cpg	1047.51	J/molxK	999.75	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=U392377&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392377&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>

# 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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