

# L-Leucine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, pentyl

Inchi:  
ester

InChI=1S/C21H41NO4/c1-7-10-12-14-25-20(23)19(15-17(4)5)22(6)21(24)26-16-18(9-3)1

InchiKey:

SQULXEDUAOYLSP-UHFFFAOYSA-N

Formula:

C21H41NO4

SMILES:

CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]:

371.55

## Physical Properties

Property code	Value	Unit	Source
gf	-238.44	kJ/mol	Joback Method
hf	-914.68	kJ/mol	Joback Method
hfus	48.17	kJ/mol	Joback Method
hvap	81.53	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.419		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpola	2162.00		NIST Webbook
rinpola	2162.00		NIST Webbook
tb	843.58	K	Joback Method
tc	1034.17	K	Joback Method
tf	458.22	K	Joback Method
vc	1.260	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.42	J/molxK	843.58	Joback Method
cpg	1094.38	J/molxK	875.35	Joback Method
cpg	1112.13	J/molxK	907.11	Joback Method
cpg	1128.71	J/molxK	938.88	Joback Method
cpg	1144.15	J/molxK	970.64	Joback Method
cpg	1158.47	J/molxK	1002.41	Joback Method
cpg	1171.70	J/molxK	1034.17	Joback Method

# Sources

<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=U392390&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392390&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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