

# L-Leucine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, undecyl ester

InChI: InChI=1S/C27H53NO4/c1-7-10-12-13-14-15-16-17-18-20-31-26(29)25(21-23(4)5)28(6)27  
InChIKey: ZCNAHFUCUZWTEGU-UHFFFAOYSA-N

Formula: C27H53NO4

SMILES: CCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 455.71

## Physical Properties

Property code	Value	Unit	Source
gf	-187.92	kJ/mol	Joback Method
hf	-1038.52	kJ/mol	Joback Method
hfus	63.71	kJ/mol	Joback Method
hvap	94.89	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.760		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	732.04	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
tb	980.86	K	Joback Method
tc	1210.38	K	Joback Method
tf	525.84	K	Joback Method
vc	1.595	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.86	J/molxK	980.86	Joback Method
cpg	1477.58	J/molxK	1019.11	Joback Method
cpg	1497.41	J/molxK	1057.37	Joback Method
cpg	1515.45	J/molxK	1095.62	Joback Method
cpg	1531.76	J/molxK	1133.87	Joback Method
cpg	1546.42	J/molxK	1172.13	Joback Method
cpg	1559.49	J/molxK	1210.38	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.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=U392394&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392394&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>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>rinpola:</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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