

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

Inchi:  
ester

InChI=1S/C25H49NO4/c1-7-10-12-13-14-15-16-18-29-24(27)23(19-21(4)5)26(6)25(28)30

InchiKey:

XUYZHGWGACKZAV-UHFFFAOYSA-N

Formula:

C25H49NO4

SMILES:

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

Mol. weight [g/mol]:

427.66

## Physical Properties

Property code	Value	Unit	Source
gf	-204.76	kJ/mol	Joback Method
hf	-997.24	kJ/mol	Joback Method
hfus	58.53	kJ/mol	Joback Method
hvap	90.43	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.980		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	814.46	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	935.10	K	Joback Method
tc	1147.35	K	Joback Method
tf	503.30	K	Joback Method
vc	1.484	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1327.15	J/molxK	935.10	Joback Method
cpg	1347.78	J/molxK	970.48	Joback Method
cpg	1366.83	J/molxK	1005.85	Joback Method
cpg	1384.34	J/molxK	1041.23	Joback Method
cpg	1400.37	J/molxK	1076.60	Joback Method
cpg	1414.98	J/molxK	1111.98	Joback Method
cpg	1428.21	J/molxK	1147.35	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=U392392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392392&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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