

# L-Leucine, N-methyl-N-(octyloxycarbonyl)-, octyl ester

Inchi:	InChI=1S/C24H47NO4/c1-6-8-10-12-14-16-18-28-23(26)22(20-21(3)4)25(5)24(27)29-19
InchiKey:	XUYGVIXUOKOCLF-JOCHJYFZSA-N
Formula:	C24H47NO4
SMILES:	CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]:	413.63

## Physical Properties

Property code	Value	Unit	Source
gf	-210.74	kJ/mol	Joback Method
hf	-971.32	kJ/mol	Joback Method
hfus	59.46	kJ/mol	Joback Method
hvap	88.60	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.734		Crippen Method
mvol	373.880	ml/mol	McGowan Method
pc	856.97	kPa	Joback Method
rinpol	3103.00		NIST Webbook
rinpol	3103.00		NIST Webbook
tb	912.66	K	Joback Method
tc	1118.65	K	Joback Method
tf	507.03	K	Joback Method
vc	1.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.02	J/mol×K	912.66	Joback Method
cpg	1283.26	J/mol×K	946.99	Joback Method
cpg	1302.04	J/mol×K	981.32	Joback Method
cpg	1319.40	J/mol×K	1015.66	Joback Method
cpg	1335.38	J/mol×K	1049.99	Joback Method
cpg	1350.03	J/mol×K	1084.32	Joback Method
cpg	1363.40	J/mol×K	1118.65	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392361&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392361&amp;Units=SI</a>
<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>

# 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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