

# L-Leucine, N-methyl-N-(hexyloxycarbonyl)-, heptadecyl ester

<b>Inchi:</b>	InChI=1S/C31H61NO4/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-22-24-25-35-30(33)29
<b>InchiKey:</b>	LZVCBZBSEUKUQE-GDLZYMKVSA-N
<b>Formula:</b>	C31H61NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	511.82

## Physical Properties

Property code	Value	Unit	Source
gf	-151.80	kJ/mol	Joback Method
hf	-1115.80	kJ/mol	Joback Method
hfus	77.59	kJ/mol	Joback Method
hvap	104.18	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	9.464		Crippen Method
mcvol	472.510	ml/mol	McGowan Method
pc	598.38	kPa	Joback Method
rinpol	3197.00		NIST Webbook
rinpol	3197.00		NIST Webbook
tb	1072.82	K	Joback Method
tc	1357.65	K	Joback Method
tf	585.92	K	Joback Method
vc	1.825	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.91	J/molxK	1072.82	Joback Method
cpg	1741.83	J/molxK	1120.29	Joback Method
cpg	1763.93	J/molxK	1167.76	Joback Method
cpg	1783.38	J/molxK	1215.23	Joback Method
cpg	1800.34	J/molxK	1262.71	Joback Method
cpg	1814.99	J/molxK	1310.18	Joback Method
cpg	1827.50	J/molxK	1357.65	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U392355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392355&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>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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