

# L-Leucine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, octyl ester

InChI: InChI=1S/C26H49NO4/c1-8-9-10-11-12-13-16-30-25(28)23(17-19(2)3)27(7)26(29)31-24

InChIKey: JKVPJVACKJOOQO-UHFFFAOYSA-N

Formula: C26H49NO4

SMILES: CCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 439.67

## Physical Properties

Property code	Value	Unit	Source
gf	-187.31	kJ/mol	Joback Method
hf	-1004.24	kJ/mol	Joback Method
hfus	55.10	kJ/mol	Joback Method
hvap	92.47	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.834		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
pc	834.83	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	968.19	K	Joback Method
tc	1185.47	K	Joback Method
tf	513.47	K	Joback Method
vc	1.470	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1396.03	J/molxK	968.19	Joback Method
cpg	1416.10	J/molxK	1004.40	Joback Method
cpg	1434.24	J/molxK	1040.62	Joback Method
cpg	1450.46	J/molxK	1076.83	Joback Method
cpg	1464.84	J/molxK	1113.05	Joback Method
cpg	1477.40	J/molxK	1149.26	Joback Method
cpg	1488.19	J/molxK	1185.47	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392415&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>
<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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