

# I-Leucine, N-ethoxycarbonyl-N-methyl-, hexadecyl ester

<b>Inchi:</b>	InChI=1S/C26H51NO4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-31-25(28)24(22-2
<b>InchiKey:</b>	BJAGRHLPGZVRQP-UHFFFAOYSA-N
<b>Formula:</b>	C26H51NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC
<b>Mol. weight [g/mol]:</b>	441.69

## Physical Properties

Property code	Value	Unit	Source
gf	-193.90	kJ/mol	Joback Method
hf	-1012.60	kJ/mol	Joback Method
hfus	64.65	kJ/mol	Joback Method
hvap	93.05	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.514		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	768.19	kPa	Joback Method
rinsol	2846.00		NIST Webbook
tb	958.42	K	Joback Method
tc	1180.17	K	Joback Method
tf	529.57	K	Joback Method
vc	1.546	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.97	J/molxK	958.42	Joback Method
cpg	1412.29	J/molxK	995.38	Joback Method
cpg	1431.89	J/molxK	1032.34	Joback Method
cpg	1449.83	J/molxK	1069.30	Joback Method
cpg	1466.16	J/molxK	1106.26	Joback Method
cpg	1480.95	J/molxK	1143.22	Joback Method
cpg	1494.27	J/molxK	1180.17	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=U321930&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321930&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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