

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

Inchi:	InChI=1S/C15H29NO4/c1-6-8-9-10-20-14(17)13(11-12(3)4)16(5)15(18)19-7-2/h12-13H,6
InchiKey:	FXSMZWUYBOKLNT-UHFFFAOYSA-N
Formula:	C15H29NO4
SMILES:	CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC
Mol. weight [g/mol]:	287.40

## Physical Properties

Property code	Value	Unit	Source
gf	-286.52	kJ/mol	Joback Method
hf	-785.56	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.223		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpola	1745.00		NIST Webbook
rinpola	1745.00		NIST Webbook
tb	706.74	K	Joback Method
tc	886.30	K	Joback Method
tf	405.60	K	Joback Method
vc	0.929	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.05	J/mol×K	706.74	Joback Method
cpg	735.81	J/mol×K	736.67	Joback Method
cpg	751.71	J/mol×K	766.59	Joback Method
cpg	766.75	J/mol×K	796.52	Joback Method
cpg	780.95	J/mol×K	826.45	Joback Method
cpg	794.33	J/mol×K	856.38	Joback Method
cpg	806.88	J/mol×K	886.30	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=U321922&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321922&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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