

# I-Leucine, N-allyloxycarbonyl-N-methyl-, hexyl ester

<b>Inchi:</b>	InChI=1S/C17H31NO4/c1-6-8-9-10-12-21-16(19)15(13-14(3)4)18(5)17(20)22-11-7-2/h7,
<b>InchiKey:</b>	YFBQFCTUIXYZLV-UHFFFAOYSA-N
<b>Formula:</b>	C17H31NO4
<b>SMILES:</b>	C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	313.43

## Physical Properties

Property code	Value	Unit	Source
gf	-181.84	kJ/mol	Joback Method
hf	-701.41	kJ/mol	Joback Method
hfus	40.05	kJ/mol	Joback Method
hvap	72.34	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.779		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinsol	1919.00		NIST Webbook
tb	749.18	K	Joback Method
tc	931.07	K	Joback Method
tf	426.38	K	Joback Method
vc	1.022	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.50	J/mol×K	749.18	Joback Method
cpg	825.48	J/mol×K	779.50	Joback Method
cpg	841.52	J/mol×K	809.81	Joback Method
cpg	856.64	J/mol×K	840.13	Joback Method
cpg	870.86	J/mol×K	870.44	Joback Method
cpg	884.21	J/mol×K	900.76	Joback Method
cpg	896.70	J/mol×K	931.07	Joback Method

# Sources

<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=U321899&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321899&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvap:</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>rinpola:</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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