

# I-Leucine, n-butoxycarbonyl-N-methyl-, hexyl ester

Inchi:	InChI=1S/C18H35NO4/c1-6-8-10-11-13-22-17(20)16(14-15(3)4)19(5)18(21)23-12-9-7-2/
InchiKey:	OXKAUQIWYMSYPZ-UHFFFAOYSA-N
Formula:	C18H35NO4
SMILES:	CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCC
Mol. weight [g/mol]:	329.47

## Physical Properties

Property code	Value	Unit	Source
gf	-261.26	kJ/mol	Joback Method
hf	-847.48	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.393		Crippen Method
mvol	289.340	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	775.38	K	Joback Method
tc	957.28	K	Joback Method
tf	439.41	K	Joback Method
vc	1.097	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.99	J/mol×K	775.38	Joback Method
cpg	910.82	J/mol×K	805.70	Joback Method
cpg	927.65	J/mol×K	836.01	Joback Method
cpg	943.49	J/mol×K	866.33	Joback Method
cpg	958.38	J/mol×K	896.65	Joback Method
cpg	972.31	J/mol×K	926.96	Joback Method
cpg	985.32	J/mol×K	957.28	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.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=U321885&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321885&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>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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