

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

Inchi:	InChI=1S/C20H39NO4/c1-6-8-10-11-12-13-15-24-19(22)18(16-17(3)4)21(5)20(23)25-14
InchiKey:	SLXXTLCHZFCXRO-UHFFFAOYSA-N
Formula:	C20H39NO4
SMILES:	CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCC
Mol. weight [g/mol]:	357.53

## Physical Properties

Property code	Value	Unit	Source
gf	-244.42	kJ/mol	Joback Method
hf	-888.76	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.173		Crippen Method
mvol	317.520	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1007.78	K	Joback Method
tf	461.95	K	Joback Method
vc	1.210	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.53	J/molxK	821.14	Joback Method
cpg	1032.07	J/molxK	852.25	Joback Method
cpg	1049.49	J/molxK	883.35	Joback Method
cpg	1065.82	J/molxK	914.46	Joback Method
cpg	1081.08	J/molxK	945.57	Joback Method
cpg	1095.30	J/molxK	976.68	Joback Method
cpg	1108.50	J/molxK	1007.78	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=U321887&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321887&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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