

# I-Leucine, N-isobutoxycarbonyl-N-methyl-, octyl ester

<b>Inchi:</b>	InChI=1S/C20H39NO4/c1-7-8-9-10-11-12-13-24-19(22)18(14-16(2)3)21(6)20(23)25-15-1
<b>InchiKey:</b>	FERXWYXZZDLKNY-UHFFFAOYSA-N
<b>Formula:</b>	C20H39NO4
<b>SMILES:</b>	CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	357.53

## Physical Properties

Property code	Value	Unit	Source
gf	-246.86	kJ/mol	Joback Method
hf	-894.04	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	5.029		Crippen Method
mvol	317.520	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
tb	820.70	K	Joback Method
tc	1008.12	K	Joback Method
tf	446.95	K	Joback Method
vc	1.204	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.01	J/molxK	820.70	Joback Method
cpg	1032.62	J/molxK	851.94	Joback Method
cpg	1050.10	J/molxK	883.17	Joback Method
cpg	1066.47	J/molxK	914.41	Joback Method
cpg	1081.75	J/molxK	945.64	Joback Method
cpg	1095.97	J/molxK	976.88	Joback Method
cpg	1109.16	J/molxK	1008.12	Joback Method

# Sources

<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=U321874&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321874&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>rlnol:</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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