

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

<b>Inchi:</b>	InChI=1S/C30H59NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-34-29(32)
<b>InchiKey:</b>	AYKJWKHVOIPLMQ-UHFFFAOYSA-N
<b>Formula:</b>	C30H59NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	497.79

## Physical Properties

Property code	Value	Unit	Source
gf	-162.66	kJ/mol	Joback Method
hf	-1100.44	kJ/mol	Joback Method
hfus	71.48	kJ/mol	Joback Method
hvap	101.56	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	8.930		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
pc	630.03	kPa	Joback Method
tb	1049.50	K	Joback Method
tc	1315.06	K	Joback Method
tf	559.65	K	Joback Method
vc	1.764	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.38	J/molxK	1049.50	Joback Method
cpg	1675.08	J/molxK	1093.76	Joback Method
cpg	1696.29	J/molxK	1138.02	Joback Method
cpg	1715.14	J/molxK	1182.28	Joback Method
cpg	1731.75	J/molxK	1226.54	Joback Method
cpg	1746.26	J/molxK	1270.80	Joback Method
cpg	1758.80	J/molxK	1315.06	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=U321881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321881&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>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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