

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

<b>Inchi:</b>	InChI=1S/C30H59NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-34-29(32)
<b>InchiKey:</b>	MBNCOGWZCOUYRJ-UHFFFAOYSA-N
<b>Formula:</b>	C30H59NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	497.79

## Physical Properties

Property code	Value	Unit	Source
gf	-160.22	kJ/mol	Joback Method
hf	-1095.16	kJ/mol	Joback Method
hfus	75.00	kJ/mol	Joback Method
hvap	101.95	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	9.074		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
pc	627.51	kPa	Joback Method
tb	1049.94	K	Joback Method
tc	1319.00	K	Joback Method
tf	574.65	K	Joback Method
vc	1.770	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.20	J/molxK	1049.94	Joback Method
cpg	1675.29	J/molxK	1094.78	Joback Method
cpg	1696.85	J/molxK	1139.63	Joback Method
cpg	1716.00	J/molxK	1184.47	Joback Method
cpg	1732.89	J/molxK	1229.31	Joback Method
cpg	1747.65	J/molxK	1274.16	Joback Method
cpg	1760.41	J/molxK	1319.00	Joback Method

# Sources

<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=U321895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321895&amp;Units=SI</a>
<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>

# 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

Latest version available from:

<https://www.chemeo.com/cid/98-914-9/l-Leucine-n-butoxycarbonyl-N-methyl-octadecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 17:55:50.973712008 +0000 UTC m=+16184199.894289322.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.