

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

<b>Inchi:</b>	InChI=1S/C29H57NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-33-28(31)27(2)
<b>InchiKey:</b>	PVKMCCGPFKKHPT-UHFFFAOYSA-N
<b>Formula:</b>	C29H57NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	483.77

## Physical Properties

Property code	Value	Unit	Source
gf	-171.08	kJ/mol	Joback Method
hf	-1079.80	kJ/mol	Joback Method
hfus	68.89	kJ/mol	Joback Method
hvap	99.34	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.540		Crippen Method
mvol	444.330	ml/mol	McGowan Method
pc	661.53	kPa	Joback Method
rinpol	3197.00		NIST Webbook
rinpol	3197.00		NIST Webbook
tb	1026.62	K	Joback Method
tc	1278.67	K	Joback Method
tf	548.38	K	Joback Method
vc	1.708	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.94	J/mol×K	1026.62	Joback Method
cpg	1608.93	J/mol×K	1068.63	Joback Method
cpg	1629.66	J/mol×K	1110.64	Joback Method
cpg	1648.23	J/mol×K	1152.64	Joback Method
cpg	1664.77	J/mol×K	1194.65	Joback Method
cpg	1679.36	J/mol×K	1236.66	Joback Method
cpg	1692.13	J/mol×K	1278.67	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=U321880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321880&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinp:</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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