

# I-Leucine, N-neopentyloxycarbonyl-N-methyl-, neopentyl ester

<b>Inchi:</b>	InChI=1S/C18H35NO4/c1-13(2)10-14(15(20)22-11-17(3,4)5)19(9)16(21)23-12-18(6,7)8/
<b>InchiKey:</b>	OCUYRQWPXLJKBP-UHFFFAOYSA-N
<b>Formula:</b>	C18H35NO4
<b>SMILES:</b>	CC(C)CC(C(=O)OCC(C)(C)C)N(C)C(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	329.47

## Physical Properties

Property code	Value	Unit	Source
gf	-255.58	kJ/mol	Joback Method
hf	-864.98	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	72.65	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.105		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
tb	768.92	K	Joback Method
tc	960.09	K	Joback Method
tf	444.25	K	Joback Method
vc	1.075	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.86	J/molxK	768.92	Joback Method
cpg	914.10	J/molxK	800.78	Joback Method
cpg	931.24	J/molxK	832.64	Joback Method
cpg	947.32	J/molxK	864.51	Joback Method
cpg	962.39	J/molxK	896.37	Joback Method
cpg	976.50	J/molxK	928.23	Joback Method
cpg	989.71	J/molxK	960.09	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=U321920&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321920&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

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