

# I-Leucine, N-neopentylloxycarbonyl-N-methyl-, pentadecyl ester

<b>Inchi:</b>	InChI=1S/C28H55NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-32-26(30)25(22-24
<b>InchiKey:</b>	GAVPSZMEXLQUAX-UHFFFAOYSA-N
<b>Formula:</b>	C28H55NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	469.74

## Physical Properties

Property code	Value	Unit	Source
gf	-174.22	kJ/mol	Joback Method
hf	-1062.63	kJ/mol	Joback Method
hfus	62.41	kJ/mol	Joback Method
hvap	96.21	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	8.150		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
tb	1000.95	K	Joback Method
tc	1236.28	K	Joback Method
tf	554.53	K	Joback Method
vc	1.647	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.05	J/molxK	1000.95	Joback Method
cpg	1542.17	J/molxK	1040.17	Joback Method
cpg	1562.50	J/molxK	1079.39	Joback Method
cpg	1581.13	J/molxK	1118.61	Joback Method
cpg	1598.17	J/molxK	1157.83	Joback Method
cpg	1613.74	J/molxK	1197.06	Joback Method
cpg	1627.94	J/molxK	1236.28	Joback Method

# Sources

<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>
<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=U321916&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321916&amp;Units=SI</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>mccvol:</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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