

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

<b>Inchi:</b>	InChI=1S/C26H51NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-30-25(28)24(20-22(2)3)
<b>InchiKey:</b>	YXXLGUJDOYAUQG-UHFFFAOYSA-N
<b>Formula:</b>	C26H51NO4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	441.69

## Physical Properties

Property code	Value	Unit	Source
gf	-196.34	kJ/mol	Joback Method
hf	-1017.88	kJ/mol	Joback Method
hfus	61.12	kJ/mol	Joback Method
hvap	92.66	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	7.370		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	771.60	kPa	Joback Method
rinpola	2751.00		NIST Webbook
tb	957.98	K	Joback Method
tc	1178.26	K	Joback Method
tf	514.57	K	Joback Method
vc	1.540	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.31	J/molxK	957.98	Joback Method
cpg	1412.46	J/molxK	994.69	Joback Method
cpg	1431.89	J/molxK	1031.41	Joback Method
cpg	1449.66	J/molxK	1068.12	Joback Method
cpg	1465.84	J/molxK	1104.83	Joback Method
cpg	1480.48	J/molxK	1141.54	Joback Method
cpg	1493.65	J/molxK	1178.26	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=U321877&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321877&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>rinpola:</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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