

# I-Leucine, N-benzyloxycarbonyl-N-methyl-, isoheptyl ester

<b>Inchi:</b>	InChI=1S/C21H33NO4/c1-16(2)10-9-13-25-20(23)19(14-17(3)4)22(5)21(24)26-15-18-11
<b>InchiKey:</b>	CXFHWECVKHOBHH-UHFFFAOYSA-N
<b>Formula:</b>	C21H33NO4
<b>SMILES:</b>	CC(C)CCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
<b>Mol. weight [g/mol]:</b>	363.49

## Physical Properties

Property code	Value	Unit	Source
gf	-126.03	kJ/mol	Joback Method
hf	-678.15	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.649		Crippen Method
mvol	307.850	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	870.26	K	Joback Method
tc	1075.29	K	Joback Method
tf	484.64	K	Joback Method
vc	1.151	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.01	J/molxK	870.26	Joback Method
cpg	998.74	J/molxK	904.43	Joback Method
cpg	1014.19	J/molxK	938.60	Joback Method
cpg	1028.42	J/molxK	972.78	Joback Method
cpg	1041.45	J/molxK	1006.95	Joback Method
cpg	1053.34	J/molxK	1041.12	Joback Method
cpg	1064.11	J/molxK	1075.29	Joback Method

# Sources

<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=U322039&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U322039&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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