

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

Inchi:	InChI=1S/C19H29NO4/c1-5-6-12-23-18(21)17(13-15(2)3)20(4)19(22)24-14-16-10-8-7-9-
InchiKey:	MCKNSDLNKOPESH-UHFFFAOYSA-N
Formula:	C19H29NO4
SMILES:	CCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]:	335.44

## Physical Properties

Property code	Value	Unit	Source
gf	-140.43	kJ/mol	Joback Method
hf	-631.59	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	79.74	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.013		Crippen Method
mvol	279.670	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rmpol	2192.00		NIST Webbook
tb	824.94	K	Joback Method
tc	1027.17	K	Joback Method
tf	477.10	K	Joback Method
vc	1.046	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.81	J/mol×K	824.94	Joback Method
cpg	879.13	J/mol×K	858.65	Joback Method
cpg	894.27	J/mol×K	892.35	Joback Method
cpg	908.28	J/mol×K	926.06	Joback Method
cpg	921.18	J/mol×K	959.76	Joback Method
cpg	933.00	J/mol×K	993.47	Joback Method
cpg	943.80	J/mol×K	1027.17	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=U322037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U322037&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>
<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>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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