

# L-Leucine, N-methyl-N-benzyloxycarbonyl-, benzyl ester

<b>Inchi:</b>	InChI=1S/C22H27NO4/c1-17(2)14-20(21(24)26-15-18-10-6-4-7-11-18)23(3)22(25)27-16
<b>InchiKey:</b>	MPXCMESMKSODDK-UHFFFAOYSA-N
<b>Formula:</b>	C22H27NO4
<b>SMILES:</b>	CC(C)CC(C(=O)OCc1ccccc1)N(C)C(=O)OCc1ccccc1
<b>Mol. weight [g/mol]:</b>	369.45

## Physical Properties

Property code	Value	Unit	Source
gf	-2.76	kJ/mol	Joback Method
hf	-456.98	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.413		Crippen Method
mvol	298.180	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2612.00		NIST Webbook
tb	920.26	K	Joback Method
tc	1144.74	K	Joback Method
tf	537.33	K	Joback Method
vc	1.105	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.03	J/mol×K	920.26	Joback Method
cpg	956.59	J/mol×K	957.67	Joback Method
cpg	969.79	J/mol×K	995.09	Joback Method
cpg	981.68	J/mol×K	1032.50	Joback Method
cpg	992.32	J/mol×K	1069.92	Joback Method
cpg	1001.79	J/mol×K	1107.33	Joback Method
cpg	1010.15	J/mol×K	1144.74	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=U322044&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U322044&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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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