

# L-Leucine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi:	InChI=1S/C14H27NO4/c1-7-18-14(17)15-12(8-9(2)3)13(16)19-11(6)10(4)5/h9-12H,7-8H2
InchiKey:	UJEQPEHLZYHWJT-JHJMLUEUSA-N
Formula:	C14H27NO4
SMILES:	CCOC(=O)NC(CC(C)C)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	273.37

## Physical Properties

Property code	Value	Unit	Source
gf	-321.21	kJ/mol	Joback Method
hf	-789.54	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.735		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	1649.80		NIST Webbook
rinpol	1649.80		NIST Webbook
tb	720.71	K	Joback Method
tc	909.23	K	Joback Method
tf	384.52	K	Joback Method
vc	0.878	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.96	J/molxK	720.71	Joback Method
cpg	699.14	J/molxK	752.13	Joback Method
cpg	714.43	J/molxK	783.55	Joback Method
cpg	728.81	J/molxK	814.97	Joback Method
cpg	742.31	J/molxK	846.39	Joback Method
cpg	754.92	J/molxK	877.81	Joback Method
cpg	766.65	J/molxK	909.23	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=R502111&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R502111&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>hvp:</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>rinp:</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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