

# L-Leucine, N-(trifluoroacetyl)-, butyl ester

<b>Other names:</b>	Leucine, N-(trifluoroacetyl)-, butyl ester, L-Leu, butyl ester, TFA, (L)-Leu, butyl ester, TFA Leu TFA Bu
<b>Inchi:</b>	InChI=1S/C12H20F3NO3/c1-4-5-6-19-10(17)9(7-8(2)3)16-11(18)12(13,14)15/h8-9H,4-7H
<b>InchiKey:</b>	HCVXJFNYPYUOKE-SECBINFHSA-N
<b>Formula:</b>	C12H20F3NO3
<b>SMILES:</b>	CCCCOC(=O)C(CC(C)C)NC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	283.29
<b>CAS:</b>	2796-38-5

## Physical Properties

Property code	Value	Unit	Source
gf	-809.76	kJ/mol	Joback Method
hf	-1202.56	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.423		Crippen Method
mcvol	204.240	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1349.00		NIST Webbook
rinpol	1349.00		NIST Webbook
tb	647.99	K	Joback Method
tc	822.24	K	Joback Method
tf	373.94	K	Joback Method
vc	0.803	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.88	J/mol×K	647.99	Joback Method
cpg	585.76	J/mol×K	677.03	Joback Method
cpg	598.90	J/mol×K	706.07	Joback Method

cpg	611.33	J/mol×K	735.12	Joback Method
cpg	623.07	J/mol×K	764.16	Joback Method
cpg	634.13	J/mol×K	793.20	Joback Method
cpg	644.55	J/mol×K	822.24	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2796385&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2796385&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>rinpolar:</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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