

# L-Leucine, N-chlorodifluoroacetyl-, ethyl ester

<b>Inchi:</b>	InChI=1S/C10H16ClF2NO3/c1-4-17-8(15)7(5-6(2)3)14-9(16)10(11,12)13/h6-7H,4-5H2,1-
<b>InchiKey:</b>	AJUCRZXKKPEULW-UHFFFAOYSA-N
<b>Formula:</b>	C10H16ClF2NO3
<b>SMILES:</b>	CCOC(=O)C(CC(C)C)NC(=O)C(F)(F)Cl
<b>Mol. weight [g/mol]:</b>	271.69

## Physical Properties

Property code	Value	Unit	Source
gf	-643.72	kJ/mol	Joback Method
hf	-980.91	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.912		Crippen Method
mvol	186.530	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
tb	640.39	K	Joback Method
tc	827.82	K	Joback Method
tf	380.73	K	Joback Method
vc	0.723	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.48	J/molxK	640.39	Joback Method
cpg	501.98	J/molxK	671.63	Joback Method
cpg	513.74	J/molxK	702.87	Joback Method
cpg	524.79	J/molxK	734.11	Joback Method
cpg	535.15	J/molxK	765.34	Joback Method
cpg	544.85	J/molxK	796.58	Joback Method
cpg	553.92	J/molxK	827.82	Joback Method

# Sources

<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=U375622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375622&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>

# 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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