

# L-Valine, N-(5-chlorovaleryl)-, isobutyl ester

<b>Inchi:</b>	InChI=1S/C14H26ClNO3/c1-10(2)9-19-14(18)13(11(3)4)16-12(17)7-5-6-8-15/h10-11,13H
<b>InchiKey:</b>	HVHZIDOMBYAFJX-UHFFFAOYSA-N
<b>Formula:</b>	C14H26ClNO3
<b>SMILES:</b>	CC(C)COC(=O)C(NC(=O)CCCCCl)C(C)C
<b>Mol. weight [g/mol]:</b>	291.81

## Physical Properties

Property code	Value	Unit	Source
gf	-225.70	kJ/mol	Joback Method
hf	-667.78	kJ/mol	Joback Method
hfus	35.13	kJ/mol	Joback Method
hvap	72.32	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.735		Crippen Method
mvol	239.350	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	736.16	K	Joback Method
tc	926.66	K	Joback Method
tf	407.21	K	Joback Method
vc	0.915	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.44	J/molxK	736.16	Joback Method
cpg	698.72	J/molxK	767.91	Joback Method
cpg	713.12	J/molxK	799.66	Joback Method
cpg	726.65	J/molxK	831.41	Joback Method
cpg	739.35	J/molxK	863.16	Joback Method
cpg	751.23	J/molxK	894.91	Joback Method
cpg	762.30	J/molxK	926.66	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=U346583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346583&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>
<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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