

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

<b>Inchi:</b>	InChI=1S/C15H28ClNO3/c1-4-5-8-11-20-15(19)14(12(2)3)17-13(18)9-6-7-10-16/h12,14H
<b>InchiKey:</b>	XHDWNENBSOXOHU-UHFFFAOYSA-N
<b>Formula:</b>	C15H28ClNO3
<b>SMILES:</b>	CCCCCOC(=O)C(NC(=O)CCCCCl)C(C)C
<b>Mol. weight [g/mol]:</b>	305.84

## Physical Properties

Property code	Value	Unit	Source
gf	-214.84	kJ/mol	Joback Method
hf	-683.14	kJ/mol	Joback Method
hfus	41.24	kJ/mol	Joback Method
hvap	74.93	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.270		Crippen Method
mvol	253.440	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	759.48	K	Joback Method
tc	947.48	K	Joback Method
tf	433.48	K	Joback Method
vc	0.978	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.07	J/mol×K	759.48	Joback Method
cpg	754.52	J/mol×K	790.81	Joback Method
cpg	769.09	J/mol×K	822.15	Joback Method
cpg	782.78	J/mol×K	853.48	Joback Method
cpg	795.64	J/mol×K	884.81	Joback Method
cpg	807.67	J/mol×K	916.15	Joback Method
cpg	818.89	J/mol×K	947.48	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U346585&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346585&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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