

# L-Phenylalanine, N-(5-chlorovaleryl)-, methyl ester

<b>Other names:</b>	L-Phenylalanine, N-(5-hlorovaleryl)-, methyl ester
<b>Inchi:</b>	InChI=1S/C15H20ClNO3/c1-20-15(19)13(11-12-7-3-2-4-8-12)17-14(18)9-5-6-10-16/h2-4
<b>InchiKey:</b>	JMOWXKQIYNSZQF-UHFFFAOYSA-N
<b>Formula:</b>	C15H20ClNO3
<b>SMILES:</b>	<chem>COC(=O)C(Cc1ccccc1)NC(=O)CCCCCl</chem>
<b>Mol. weight [g/mol]:</b>	297.78

## Physical Properties

Property code	Value	Unit	Source
gf	-99.99	kJ/mol	Joback Method
hf	-441.33	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.296		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	2189.00		NIST Webbook
tb	786.60	K	Joback Method
tc	998.08	K	Joback Method
tf	474.90	K	Joback Method
vc	0.875	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.87	J/mol×K	786.60	Joback Method
cpg	662.52	J/mol×K	821.85	Joback Method
cpg	675.17	J/mol×K	857.09	Joback Method
cpg	686.85	J/mol×K	892.34	Joback Method
cpg	697.60	J/mol×K	927.59	Joback Method
cpg	707.45	J/mol×K	962.84	Joback Method
cpg	716.44	J/mol×K	998.08	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=U299719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299719&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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