

# L-Phenylalanine, N-pivaloyl-, methyl ester

<b>Inchi:</b>	InChI=1S/C15H21NO3/c1-15(2,3)14(18)16-12(13(17)19-4)10-11-8-6-5-7-9-11/h5-9,12H,
<b>InchiKey:</b>	HKQYJNOOHJMWEY-UHFFFAOYSA-N
<b>Formula:</b>	C15H21NO3
<b>SMILES:</b>	COC(=O)C(Cc1ccccc1)NC(=O)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	263.33

## Physical Properties

Property code	Value	Unit	Source
gf	-85.22	kJ/mol	Joback Method
hf	-434.34	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	71.91	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.933		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpola	1772.00		NIST Webbook
rinpola	1772.00		NIST Webbook
tb	745.94	K	Joback Method
tc	963.54	K	Joback Method
tf	447.40	K	Joback Method
vc	0.816	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.13	J/molxK	745.94	Joback Method
cpg	640.33	J/molxK	782.21	Joback Method
cpg	654.41	J/molxK	818.47	Joback Method
cpg	667.43	J/molxK	854.74	Joback Method
cpg	679.44	J/molxK	891.01	Joback Method
cpg	690.51	J/molxK	927.28	Joback Method
cpg	700.70	J/molxK	963.54	Joback Method

# Sources

<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=U299748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299748&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>

# 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>rlnol:</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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