

# L-Phenylalanine, N-(trifluoroacetyl)-, methyl ester

<b>Other names:</b>	Alanine, 3-phenyl-N-(trifluoroacetyl)-, methyl ester, L- Alanine, 3-phenyl-N-(trifluoroacetyl)-, methyl ester Trifluoroacetyl-L-phenylalanine methyl ester N-Trifluoroacetyl-L-phenylalanine methyl ester Phe, N-TFA, methyl ester, (L)- Phe, N-TFA, methyl ester
<b>Inchi:</b>	InChI=1S/C12H12F3NO3/c1-19-10(17)9(16-11(18)12(13,14)15)7-8-5-3-2-4-6-8/h2-6,9H,
<b>InchiKey:</b>	ZYMGRJXIRUWDLX-SECBINFHSA-N
<b>Formula:</b>	C12H12F3NO3
<b>SMILES:</b>	<chem>COC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)F</chem>
<b>Mol. weight [g/mol]:</b>	275.22
<b>CAS:</b>	23635-30-5

## Physical Properties

Property code	Value	Unit	Source
gf	-694.91	kJ/mol	Joback Method
hf	-960.75	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.449		Crippen Method
mcvol	180.480	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	675.11	K	Joback Method
tc	876.35	K	Joback Method
tf	415.36	K	Joback Method
vc	0.702	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.60	J/mol×K	675.11	Joback Method
cpg	502.88	J/mol×K	708.65	Joback Method
cpg	514.27	J/mol×K	742.19	Joback Method
cpg	524.81	J/mol×K	775.73	Joback Method
cpg	534.54	J/mol×K	809.27	Joback Method
cpg	543.50	J/mol×K	842.81	Joback Method
cpg	551.74	J/mol×K	876.35	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=C23635305&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23635305&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>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>rinpol:</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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