

# L-Tyrosine, N-(trifluoroacetyl)-, butyl ester, trifluoroacetate (ester)

<b>Other names:</b>	Tyrosine, N-(trifluoroacetyl)-, butyl ester, trifluoroacetate (ester), L-Tyr, butyl ester, N(O)-TFA Tyr, butyl ester, N-TFA Tyr TFA Bu
<b>Inchi:</b>	InChI=1S/C17H17F6NO5/c1-2-3-8-28-13(25)12(24-14(26)16(18,19)20)9-10-4-6-11(7-5-1
<b>InchiKey:</b>	BFQHENRWMAGCOB-GFCCVEGCSA-N
<b>Formula:</b>	C17H17F6NO5
<b>SMILES:</b>	CCCCOC(=O)C(Cc1ccc(OC(=O)C(F)(F)F)cc1)NC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	429.31
<b>CAS:</b>	5282-98-4

## Physical Properties

Property code	Value	Unit	Source
gf	-1477.95	kJ/mol	Joback Method
hf	-1917.30	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	79.99	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.087		Crippen Method
mcvol	263.680	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
tb	865.36	K	Joback Method
tc	1063.81	K	Joback Method
tf	560.58	K	Joback Method
vc	1.048	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.34	J/molxK	865.36	Joback Method
cpg	833.38	J/molxK	898.43	Joback Method
cpg	843.48	J/molxK	931.51	Joback Method
cpg	852.70	J/molxK	964.58	Joback Method
cpg	861.09	J/molxK	997.66	Joback Method

cpg	868.70	J/mol×K	1030.73	Joback Method
cpg	875.59	J/mol×K	1063.81	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=C5282984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5282984&amp;Units=SI</a>
<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>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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