

# L-Tyrosine, N,O-bis(2,3,4-trifluorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C24H15F6NO5/c1-35-24(34)17(31-22(32)13-6-8-15(25)20(29)18(13)27)10-11-
<b>InchiKey:</b>	BBDNFWXBCYKNCP-UHFFFAOYSA-N
<b>Formula:</b>	C24H15F6NO5
<b>SMILES:</b>	COC(=O)C(Cc1ccc(OC(=O)c2ccc(F)c(F)c2F)cc1)NC(=O)c1ccc(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	511.37

## Physical Properties

Property code	Value	Unit	Source
gf	-1257.65	kJ/mol	Joback Method
hf	-1640.04	kJ/mol	Joback Method
hfus	64.55	kJ/mol	Joback Method
hvap	106.68	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	4.255		Crippen Method
mcvol	314.790	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
tb	1115.22	K	Joback Method
tc	1365.96	K	Joback Method
tf	762.59	K	Joback Method
vc	1.246	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.46	J/molxK	1115.22	Joback Method
cpg	993.81	J/molxK	1157.01	Joback Method
cpg	997.46	J/molxK	1198.80	Joback Method
cpg	999.44	J/molxK	1240.59	Joback Method
cpg	999.79	J/molxK	1282.38	Joback Method
cpg	998.53	J/molxK	1324.17	Joback Method
cpg	995.72	J/molxK	1365.96	Joback Method

# Sources

<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>
<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=U299636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299636&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>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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