

# L-Tyrosine, N,O-bis(3-fluorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C24H19F2NO5/c1-31-24(30)21(27-22(28)16-4-2-6-18(25)13-16)12-15-8-10-20
<b>InchiKey:</b>	BDTBDTZRXWVLY-UHFFFAOYSA-N
<b>Formula:</b>	C24H19F2NO5
<b>SMILES:</b>	<chem>COC(=O)C(Cc1ccc(OC(=O)c2cccc(F)c2)cc1)NC(=O)c1cccc(F)c1</chem>
<b>Mol. weight [g/mol]:</b>	439.41

## Physical Properties

Property code	Value	Unit	Source
gf	-439.89	kJ/mol	Joback Method
hf	-809.72	kJ/mol	Joback Method
hfus	53.78	kJ/mol	Joback Method
hvap	107.30	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	3.698		Crippen Method
mcvol	307.710	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	1098.22	K	Joback Method
tc	1348.59	K	Joback Method
tf	710.15	K	Joback Method
vc	1.175	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.72	J/molxK	1098.22	Joback Method
cpg	978.91	J/molxK	1139.95	Joback Method
cpg	984.61	J/molxK	1181.68	Joback Method
cpg	988.88	J/molxK	1223.41	Joback Method
cpg	991.78	J/molxK	1265.13	Joback Method
cpg	993.39	J/molxK	1306.86	Joback Method
cpg	993.78	J/molxK	1348.59	Joback Method

# Sources

<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=U299682&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299682&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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