

# L-Tyrosine, N,O-bis(2,6-difluorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C24H17F4NO5/c1-33-23(31)19(29-22(30)20-15(25)4-2-5-16(20)26)12-13-8-10
<b>InchiKey:</b>	OEONJOSRYODGNS-UHFFFAOYSA-N
<b>Formula:</b>	C24H17F4NO5
<b>SMILES:</b>	COC(=O)C(Cc1ccc(OC(=O)c2c(F)cccc2F)cc1)NC(=O)c1c(F)cccc1F
<b>Mol. weight [g/mol]:</b>	475.39

## Physical Properties

Property code	Value	Unit	Source
gf	-848.77	kJ/mol	Joback Method
hf	-1224.88	kJ/mol	Joback Method
hfus	59.16	kJ/mol	Joback Method
hvap	106.99	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	3.976		Crippen Method
mcvol	311.250	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
tb	1106.72	K	Joback Method
tc	1355.32	K	Joback Method
tf	736.37	K	Joback Method
vc	1.210	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.23	J/molxK	1106.72	Joback Method
cpg	986.49	J/molxK	1148.15	Joback Method
cpg	991.17	J/molxK	1189.59	Joback Method
cpg	994.32	J/molxK	1231.02	Joback Method
cpg	996.00	J/molxK	1272.45	Joback Method
cpg	996.26	J/molxK	1313.89	Joback Method
cpg	995.16	J/molxK	1355.32	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299667&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299667&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>
<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>

# 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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