

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

**Inchi:** InChI=1S/C22H33NO5/c1-4-6-8-10-20(24)23-19(22(26)27-3)16-17-12-14-18(15-13-17)2  
**InchiKey:** BCGBTZOAIWRNEC-UHFFFAOYSA-N  
**Formula:** C22H33NO5  
**SMILES:** CCCCCC(=O)NC(Cc1ccc(OC(=O)CCCCC)cc1)C(=O)OC  
**Mol. weight [g/mol]:** 391.50

## Physical Properties

Property code	Value	Unit	Source
gf	-272.67	kJ/mol	Joback Method
hf	-826.34	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	98.61	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.953		Crippen Method
mcvol	323.510	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinsol	3143.00		NIST Webbook
tb	990.60	K	Joback Method
tc	1213.12	K	Joback Method
tf	608.55	K	Joback Method
vc	1.242	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.64	J/molxK	990.60	Joback Method
cpg	1084.33	J/molxK	1027.69	Joback Method
cpg	1096.57	J/molxK	1064.77	Joback Method
cpg	1107.40	J/molxK	1101.86	Joback Method
cpg	1116.85	J/molxK	1138.94	Joback Method
cpg	1124.97	J/molxK	1176.03	Joback Method
cpg	1131.79	J/molxK	1213.12	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299740&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>
<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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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