

# L-Alanine, N-(m-anisoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C12H15NO4/c1-8(12(15)17-3)13-11(14)9-5-4-6-10(7-9)16-2/h4-8H,1-3H3,(H,1
<b>InchiKey:</b>	LDWSXTOSDPJTCB-UHFFFAOYSA-N
<b>Formula:</b>	C12H15NO4
<b>SMILES:</b>	COC(=O)C(C)NC(=O)c1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	237.25

## Physical Properties

Property code	Value	Unit	Source
gf	-227.95	kJ/mol	Joback Method
hf	-507.36	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	69.60	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	0.986		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinsol	1889.00		NIST Webbook
tb	707.93	K	Joback Method
tc	923.05	K	Joback Method
tf	445.92	K	Joback Method
vc	0.676	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.91	J/mol×K	707.93	Joback Method
cpg	501.12	J/mol×K	743.78	Joback Method
cpg	513.42	J/mol×K	779.64	Joback Method
cpg	524.82	J/mol×K	815.49	Joback Method
cpg	535.31	J/mol×K	851.35	Joback Method
cpg	544.91	J/mol×K	887.20	Joback Method
cpg	553.62	J/mol×K	923.05	Joback Method

# Sources

<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=U299706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299706&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>

# 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>rinpola:</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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