

# L-Alanine, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi:	InChI=1S/C12H21NO3/c1-9(12(15)16-2)13-11(14)8-7-10-5-3-4-6-10/h9-10H,3-8H2,1-2H1
InchiKey:	ZUFRPVZUKJBNJQ-UHFFFAOYSA-N
Formula:	C12H21NO3
SMILES:	COC(=O)C(C)N=C(O)CCC1CCCC1
Mol. weight [g/mol]:	227.30

## Physical Properties

Property code	Value	Unit	Source
hf	-560.41	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.475		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	733.83	K	Joback Method
tc	936.30	K	Joback Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299651&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299651&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

hf:	Enthalpy of formation at standard conditions
hvap:	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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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