

# «beta»-Alanine, N-cyclohexylcarbonyl-, pentyl ester

Inchi:	InChI=1S/C15H27NO3/c1-2-3-7-12-19-14(17)10-11-16-15(18)13-8-5-4-6-9-13/h13H,2-12
InchiKey:	VZQAAACBNFTVGM-UHFFFAOYSA-N
Formula:	C15H27NO3
SMILES:	CCCCCOC(=O)CCNC(=O)C1CCCCC1
Mol. weight [g/mol]:	269.38

## Physical Properties

Property code	Value	Unit	Source
gf	-173.58	kJ/mol	Joback Method
hf	-602.52	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.806		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	742.48	K	Joback Method
tc	942.55	K	Joback Method
tf	440.94	K	Joback Method
vc	0.874	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.77	J/mol×K	742.48	Joback Method
cpg	720.50	J/mol×K	775.82	Joback Method
cpg	737.10	J/mol×K	809.17	Joback Method
cpg	752.61	J/mol×K	842.51	Joback Method
cpg	767.03	J/mol×K	875.86	Joback Method
cpg	780.40	J/mol×K	909.20	Joback Method
cpg	792.75	J/mol×K	942.55	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321962&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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