

# «beta»-Alanine, N-(cyclopentylpropionyl)-, pentyl ester

Inchi:	InChI=1S/C16H29NO3/c1-2-3-6-13-20-16(19)11-12-17-15(18)10-9-14-7-4-5-8-14/h14H,2
InchiKey:	LNWWNMMMEIYEDE-UHFFFAOYSA-N
Formula:	C16H29NO3
SMILES:	CCCCCOC(=O)CCNC(=O)CCC1CCCC1
Mol. weight [g/mol]:	283.41

## Physical Properties

Property code	Value	Unit	Source
gf	-153.06	kJ/mol	Joback Method
hf	-617.00	kJ/mol	Joback Method
hfus	40.62	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.196		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpul	2247.00		NIST Webbook
rinpul	2247.00		NIST Webbook
tb	761.09	K	Joback Method
tc	955.61	K	Joback Method
tf	455.73	K	Joback Method
vc	0.938	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.67	J/mol×K	761.09	Joback Method
cpg	774.08	J/mol×K	793.51	Joback Method
cpg	790.43	J/mol×K	825.93	Joback Method
cpg	805.75	J/mol×K	858.35	Joback Method
cpg	820.09	J/mol×K	890.77	Joback Method
cpg	833.46	J/mol×K	923.19	Joback Method
cpg	845.91	J/mol×K	955.61	Joback Method

# Sources

<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=U321753&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321753&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>

# 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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