

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

<b>Inchi:</b>	InChI=1S/C25H47NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-22-29-24(27)20-21-26-25(28)
<b>InchiKey:</b>	LIDWLEXWMNSRNJ-UHFFFAOYSA-N
<b>Formula:</b>	C25H47NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)C1CCCCC1
<b>Mol. weight [g/mol]:</b>	409.65

## Physical Properties

Property code	Value	Unit	Source
gf	-89.38	kJ/mol	Joback Method
hf	-808.92	kJ/mol	Joback Method
hfus	61.83	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.707		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
tb	971.28	K	Joback Method
tc	1189.62	K	Joback Method
tf	553.64	K	Joback Method
vc	1.433	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1312.05	J/molxK	971.28	Joback Method
cpg	1331.59	J/molxK	1007.67	Joback Method
cpg	1349.50	J/molxK	1044.06	Joback Method
cpg	1365.86	J/molxK	1080.45	Joback Method
cpg	1380.74	J/molxK	1116.84	Joback Method
cpg	1394.21	J/molxK	1153.23	Joback Method
cpg	1406.32	J/molxK	1189.62	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=U321970&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321970&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>

# 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>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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