

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

Inchi:	InChI=1S/C22H41NO3/c1-2-3-4-5-6-7-8-9-10-14-19-26-21(24)17-18-23-22(25)20-15-12-
InchiKey:	ILBVEVIOYSBIPW-UHFFFAOYSA-N
Formula:	C22H41NO3
SMILES:	CCCCCCCCCCCCOC(=O)CCN=C(O)C1CCCCC1
Mol. weight [g/mol]:	367.57

## Physical Properties

Property code	Value	Unit	Source
hf	-767.69	kJ/mol	Joback Method
hvap	94.22	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.377		Crippen Method
mcvol	328.970	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2913.00		NIST Webbook
rinpol	2913.00		NIST Webbook
tb	967.34	K	Joback Method
tc	1184.34	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=U321968&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321968&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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