

# «beta»-Alanine, N-capryloyl-, decyl ester

**Inchi:** InChI=1S/C21H41NO3/c1-3-5-7-9-10-11-13-15-19-25-21(24)17-18-22-20(23)16-14-12-8  
**InchiKey:** KHCFPBDIEVLIML-UHFFFAOYSA-N  
**Formula:** C<sub>21</sub>H<sub>41</sub>NO<sub>3</sub>  
**SMILES:** CCCCCCCCCOC(=O)CCN=C(O)CCCCCCC  
**Mol. weight [g/mol]:** 355.56

## Physical Properties

Property code	Value	Unit	Source
hf	-801.37	kJ/mol	Joback Method
hvap	91.57	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.377		Crippen Method
mcvol	325.740	ml/mol	McGowan Method
pc	979.01	kPa	Joback Method
rinpol	2678.00		NIST Webbook
rinpol	2678.00		NIST Webbook
tb	924.91	K	Joback Method
tc	1133.87	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321816&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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