

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

**Inchi:** InChI=1S/C26H51NO3/c1-3-5-7-9-10-11-12-13-14-15-16-18-20-24-30-26(29)22-23-27-29  
**InchiKey:** VETVELPFRBGHAHZ-UHFFFAOYSA-N  
**Formula:** C26H51NO3  
**SMILES:** CCCCCCCCCCCCCCOC(=O)CCN=C(O)CCCCCCC  
**Mol. weight [g/mol]:** 425.69

## Physical Properties

Property code	Value	Unit	Source
hf	-904.57	kJ/mol	Joback Method
hvap	102.70	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	8.328		Crippen Method
mcvol	396.190	ml/mol	McGowan Method
pc	740.03	kPa	Joback Method
tb	1039.31	K	Joback Method
tc	1298.29	K	Joback Method

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321819&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume  
**pc:** Critical Pressure  
**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature

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