

# 2-Aminopent-4-enoic acid, N-(2-ethylhexyloxycarbonyl)-, tridecyl ester

**Inchi:** InChI=1S/C27H51NO4/c1-5-9-11-12-13-14-15-16-17-18-19-22-31-26(29)25(20-7-3)28-2  
**InchiKey:** ILMMGMYQLSYJNV-UHFFFAOYSA-N  
**Formula:** C27H51NO4  
**SMILES:** C=CCC(N=C(O)OCC(CC)CCCC)C(=O)OCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 453.70

## Physical Properties

Property code	Value	Unit	Source
hf	-942.56	kJ/mol	Joback Method
hvap	105.89	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.932		Crippen Method
mcvol	411.850	ml/mol	McGowan Method
pc	718.37	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	1080.41	K	Joback Method
tc	1355.20	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393168&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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