

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

**Inchi:** InChI=1S/C19H35NO4/c1-5-9-11-14-23-18(21)17(12-7-3)20-19(22)24-15-16(8-4)13-10-6  
**InchiKey:** XIHDCTKUTUVA AZ-UHFFFAOYSA-N  
**Formula:** C<sub>19</sub>H<sub>35</sub>NO<sub>4</sub>  
**SMILES:** C=CCC(N=C(O)OCC(CC)CCCC)C(=O)OCCCC  
**Mol. weight [g/mol]:** 341.49

## Physical Properties

Property code	Value	Unit	Source
hf	-777.44	kJ/mol	Joback Method
hvap	88.08	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.812		Crippen Method
mcvol	299.130	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	897.37	K	Joback Method
tc	1098.80	K	Joback Method

## Sources

**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=U393161&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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