

# 2-Aminopent-4-enoic acid, N-(but-3-en-1-yloxycarbonyl)-, octyl ester

**Inchi:** InChI=1S/C18H31NO4/c1-4-7-9-10-11-12-15-22-17(20)16(13-6-3)19-18(21)23-14-8-5-2/  
**InchiKey:** YMQZUUMCUHIGOZ-UHFFFAOYSA-N  
**Formula:** C18H31NO4  
**SMILES:** C=CCCOC(O)=NC(CC=C)C(=O)OCCCCCCCC  
**Mol. weight [g/mol]:** 325.44

## Physical Properties

Property code	Value	Unit	Source
hf	-626.09	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.341		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	871.61	K	Joback Method
tc	1068.41	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=U393202&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

<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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