

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

Inchi:  
ester

InChI=1S/C14H21NO4/c1-4-7-10-18-13(16)12(9-6-3)15-14(17)19-11-8-5-2/h4-6,12H,1-3

InchiKey:

YZQNATNOGQPXKY-UHFFFAOYSA-N

Formula:

C14H21NO4

SMILES:

C=CCCOC(=O)NC(CC=C)C(=O)OCCC=C

Mol. weight [g/mol]:

267.32

## Physical Properties

Property code	Value	Unit	Source
gf	-50.37	kJ/mol	Joback Method
hf	-397.41	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.353		Crippen Method
mcvol	220.080	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpola	1742.00		NIST Webbook
rinpola	1742.00		NIST Webbook
tb	712.07	K	Joback Method
tc	899.94	K	Joback Method
tf	424.24	K	Joback Method
vc	0.840	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.43	J/mol×K	712.07	Joback Method
cpg	622.35	J/mol×K	743.38	Joback Method
cpg	635.50	J/mol×K	774.69	Joback Method
cpg	647.87	J/mol×K	806.01	Joback Method
cpg	659.51	J/mol×K	837.32	Joback Method
cpg	670.41	J/mol×K	868.63	Joback Method
cpg	680.59	J/mol×K	899.94	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393207&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	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>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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