

# DL-Alanine, N-methyl-N-(but-4-en-1-yloxycarbonyl)-, octyl

InChI:  
ester

InChI=1S/C17H31NO4/c1-5-7-9-10-11-12-14-21-16(19)15(3)18(4)17(20)22-13-8-6-2/h6,

InChIKey:

AELBTEKYZMXDCW-UHFFFAOYSA-N

Formula:

C17H31NO4

SMILES:

C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCC

Mol. weight [g/mol]:

313.43

## Physical Properties

Property code	Value	Unit	Source
gf	-179.40	kJ/mol	Joback Method
hf	-696.13	kJ/mol	Joback Method
hfus	43.58	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.923		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	2026.00		NIST Webbook
rinpol	2026.00		NIST Webbook
tb	749.62	K	Joback Method
tc	929.82	K	Joback Method
tf	441.38	K	Joback Method
vc	1.028	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.01	J/molxK	749.62	Joback Method
cpg	824.81	J/molxK	779.65	Joback Method
cpg	840.71	J/molxK	809.69	Joback Method
cpg	855.71	J/molxK	839.72	Joback Method
cpg	869.83	J/molxK	869.75	Joback Method
cpg	883.11	J/molxK	899.79	Joback Method
cpg	895.55	J/molxK	929.82	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U392733&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392733&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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

Latest version available from:

<https://www.chemeo.com/cid/93-219-6/DL-Alanine-N-methyl-N-but-4-en-1-yloxycarbonyl-octyl-ester.pdf>

Generated by Cheméo on 2024-04-20 05:46:23.852765433 +0000 UTC m=+15881232.773342756.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.