

# DL-Alanine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, octyl

Inchi:  
ester

InChI=1S/C21H41NO4/c1-6-9-11-12-13-14-16-25-20(23)18(4)22(5)21(24)26-17-19(8-3)1

InchiKey:

LJGJZZWCQLETGT-UHFFFAOYSA-N

Formula:

C21H41NO4

SMILES:

CCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]:

371.55

## Physical Properties

Property code	Value	Unit	Source
gf	-236.00	kJ/mol	Joback Method
hf	-909.40	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.563		Crippen Method
mvol	331.610	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	844.02	K	Joback Method
tc	1034.17	K	Joback Method
tf	473.22	K	Joback Method
vc	1.266	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.95	J/molxK	844.02	Joback Method
cpg	1093.87	J/molxK	875.71	Joback Method
cpg	1111.61	J/molxK	907.40	Joback Method
cpg	1128.18	J/molxK	939.09	Joback Method
cpg	1143.62	J/molxK	970.78	Joback Method
cpg	1157.96	J/molxK	1002.48	Joback Method
cpg	1171.23	J/molxK	1034.17	Joback Method

# Sources

<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=U392659&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392659&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rlnol:</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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