

# D-Alanine, N-ethoxycarbonyl-, pentyl ester

<b>Inchi:</b>	InChI=1S/C11H21NO4/c1-4-6-7-8-16-10(13)9(3)12-11(14)15-5-2/h9H,4-8H2,1-3H3,(H,12)
<b>InchiKey:</b>	ZKVSNJAWCFKQHT-UHFFFAOYSA-N
<b>Formula:</b>	C11H21NO4
<b>SMILES:</b>	CCCCCOC(=O)C(C)NC(=O)OCC
<b>Mol. weight [g/mol]:</b>	231.29

## Physical Properties

Property code	Value	Unit	Source
gf	-339.15	kJ/mol	Joback Method
hf	-711.78	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.854		Crippen Method
mcvol	190.710	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
tb	653.39	K	Joback Method
tc	837.00	K	Joback Method
tf	395.71	K	Joback Method
vc	0.729	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.38	J/mol×K	653.39	Joback Method
cpg	533.47	J/mol×K	683.99	Joback Method
cpg	546.88	J/mol×K	714.59	Joback Method
cpg	559.61	J/mol×K	745.20	Joback Method
cpg	571.67	J/mol×K	775.80	Joback Method
cpg	583.04	J/mol×K	806.40	Joback Method
cpg	593.74	J/mol×K	837.00	Joback Method

# Sources

<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=U347747&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347747&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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