

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

<b>Inchi:</b>	InChI=1S/C13H25NO4/c1-4-6-7-8-9-10-18-12(15)11(3)14-13(16)17-5-2/h11H,4-10H2,1-3
<b>InchiKey:</b>	MLBJUTHIZUXARJ-UHFFFAOYSA-N
<b>Formula:</b>	C13H25NO4
<b>SMILES:</b>	CCCCCCCOC(=O)C(C)NC(=O)OCC
<b>Mol. weight [g/mol]:</b>	259.34

## Physical Properties

Property code	Value	Unit	Source
gf	-322.31	kJ/mol	Joback Method
hf	-753.06	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.635		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinsol	1761.00		NIST Webbook
tb	699.15	K	Joback Method
tc	881.01	K	Joback Method
tf	418.25	K	Joback Method
vc	0.841	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.17	J/molxK	699.15	Joback Method
cpg	641.27	J/molxK	729.46	Joback Method
cpg	655.61	J/molxK	759.77	Joback Method
cpg	669.18	J/molxK	790.08	Joback Method
cpg	681.98	J/molxK	820.39	Joback Method
cpg	694.03	J/molxK	850.70	Joback Method
cpg	705.33	J/molxK	881.01	Joback Method

# Sources

<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.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=U347750&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347750&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>hvap:</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>mccvol:</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
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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