

# D-Alanine, N-butoxycarbonyl-, nonyl ester

<b>Inchi:</b>	InChI=1S/C17H33NO4/c1-4-6-8-9-10-11-12-14-21-16(19)15(3)18-17(20)22-13-7-5-2/h15
<b>InchiKey:</b>	FFXFLSDLPLEVMM-UHFFFAOYSA-N
<b>Formula:</b>	C17H33NO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(C)NC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	315.45

## Physical Properties

Property code	Value	Unit	Source
gf	-288.63	kJ/mol	Joback Method
hf	-835.62	kJ/mol	Joback Method
hfus	46.94	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.195		Crippen Method
mvol	275.250	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	790.67	K	Joback Method
tc	975.04	K	Joback Method
tf	463.33	K	Joback Method
vc	1.065	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.75	J/mol×K	790.67	Joback Method
cpg	870.46	J/mol×K	821.40	Joback Method
cpg	886.20	J/mol×K	852.13	Joback Method
cpg	900.99	J/mol×K	882.86	Joback Method
cpg	914.84	J/mol×K	913.59	Joback Method
cpg	927.76	J/mol×K	944.31	Joback Method
cpg	939.76	J/mol×K	975.04	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=U347723&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347723&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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