

# L-Norvaline, n-butoxycarbonyl-, octyl ester

<b>Inchi:</b>	InChI=1S/C18H35NO4/c1-4-7-9-10-11-12-15-22-17(20)16(13-6-3)19-18(21)23-14-8-5-2/
<b>InchiKey:</b>	DKAFIYFGRXDWDP-UHFFFAOYSA-N
<b>Formula:</b>	C18H35NO4
<b>SMILES:</b>	CCCCCCCCOC(=O)C(CCC)NC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	329.47

## Physical Properties

Property code	Value	Unit	Source
gf	-280.21	kJ/mol	Joback Method
hf	-856.26	kJ/mol	Joback Method
hfus	49.53	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.585		Crippen Method
mvol	289.340	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	1996.00		NIST Webbook
tb	813.55	K	Joback Method
tc	1000.12	K	Joback Method
tf	474.60	K	Joback Method
vc	1.121	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.06	J/mol×K	813.55	Joback Method
cpg	930.15	J/mol×K	844.64	Joback Method
cpg	946.21	J/mol×K	875.74	Joback Method
cpg	961.26	J/mol×K	906.83	Joback Method
cpg	975.31	J/mol×K	937.93	Joback Method
cpg	988.37	J/mol×K	969.02	Joback Method
cpg	1000.48	J/mol×K	1000.12	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320776&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320776&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

# 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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