

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

<b>Inchi:</b>	InChI=1S/C22H43NO4/c1-4-7-9-10-11-12-13-14-15-16-19-26-21(24)20(17-6-3)23-22(25)
<b>InchiKey:</b>	QRRKJKCIFCFFBS-UHFFFAOYSA-N
<b>Formula:</b>	C22H43NO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	385.58

## Physical Properties

Property code	Value	Unit	Source
gf	-246.53	kJ/mol	Joback Method
hf	-938.82	kJ/mol	Joback Method
hfus	59.89	kJ/mol	Joback Method
hvap	88.93	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.146		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
tb	905.07	K	Joback Method
tc	1108.48	K	Joback Method
tf	519.68	K	Joback Method
vc	1.345	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.76	J/molxK	905.07	Joback Method
cpg	1176.49	J/molxK	938.97	Joback Method
cpg	1193.86	J/molxK	972.87	Joback Method
cpg	1209.90	J/molxK	1006.78	Joback Method
cpg	1224.64	J/molxK	1040.68	Joback Method
cpg	1238.12	J/molxK	1074.58	Joback Method
cpg	1250.36	J/molxK	1108.48	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320779&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>
<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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/68-014-1/l-Norvaline-n-butoxycarbonyl-dodecyl-ester.pdf>

Generated by Cheméo on 2024-08-09 01:47:30.319814433 +0000 UTC m=+1857919.566919779.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.