

# L-Norvaline, N-(but-2-yn-1-yloxycarbonyl)-, hexyl ester

<b>Inchi:</b>	InChI=1S/C16H27NO4/c1-4-7-9-10-13-20-15(18)14(11-6-3)17-16(19)21-12-8-5-2/h14H,4
<b>InchiKey:</b>	DYMGPVRWKSWHJQ-CQSZACIVSA-N
<b>Formula:</b>	C16H27NO4
<b>SMILES:</b>	CC#CCOC(=O)NC(CCC)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	297.39

## Physical Properties

Property code	Value	Unit	Source
gf	-94.25	kJ/mol	Joback Method
hf	-542.68	kJ/mol	Joback Method
hfus	47.47	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.028		Crippen Method
mvol	252.560	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	776.79	K	Joback Method
tc	970.94	K	Joback Method
tf	558.16	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.18	J/molxK	776.79	Joback Method
cpg	762.80	J/molxK	809.15	Joback Method
cpg	777.49	J/molxK	841.51	Joback Method
cpg	791.25	J/molxK	873.87	Joback Method
cpg	804.08	J/molxK	906.23	Joback Method
cpg	816.00	J/molxK	938.58	Joback Method
cpg	827.01	J/molxK	970.94	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392863&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.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>
<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>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>rinp:</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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