

# L-Norvaline, N-hexyloxycarbonyl-, isobutyl ester

Inchi:	InChI=1S/C16H31NO4/c1-5-7-8-9-11-20-16(19)17-14(10-6-2)15(18)21-12-13(3)4/h13-14
InchiKey:	RASRTLAPFQGSOF-CQSZACIVSA-N
Formula:	C16H31NO4
SMILES:	CCCCCCOC(=O)NC(CCC)C(=O)OCC(C)C
Mol. weight [g/mol]:	301.42

## Physical Properties

Property code	Value	Unit	Source
gf	-299.49	kJ/mol	Joback Method
hf	-820.26	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	75.18	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.661		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	767.35	K	Joback Method
tc	951.81	K	Joback Method
tf	437.06	K	Joback Method
vc	1.002	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.83	J/molxK	767.35	Joback Method
cpg	812.32	J/molxK	798.09	Joback Method
cpg	827.87	J/molxK	828.84	Joback Method
cpg	842.49	J/molxK	859.58	Joback Method
cpg	856.20	J/molxK	890.33	Joback Method
cpg	869.00	J/molxK	921.07	Joback Method
cpg	880.90	J/molxK	951.81	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392831&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392831&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>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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