

# I-Norvaline, N-methoxycarbonyl-, nonyl ester

<b>Inchi:</b>	InChI=1S/C16H31NO4/c1-4-6-7-8-9-10-11-13-21-15(18)14(12-5-2)17-16(19)20-3/h14H,4
<b>InchiKey:</b>	MDRGZXXXQZSGED-UHFFFAOYSA-N
<b>Formula:</b>	C16H31NO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CCC)NC(=O)OC
<b>Mol. weight [g/mol]:</b>	301.42

## Physical Properties

Property code	Value	Unit	Source
gf	-297.05	kJ/mol	Joback Method
hf	-814.98	kJ/mol	Joback Method
hfus	44.35	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.805		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinsol	1875.00		NIST Webbook
tb	767.79	K	Joback Method
tc	950.65	K	Joback Method
tf	452.06	K	Joback Method
vc	1.008	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.32	J/mol×K	767.79	Joback Method
cpg	811.65	J/mol×K	798.27	Joback Method
cpg	827.08	J/mol×K	828.74	Joback Method
cpg	841.60	J/mol×K	859.22	Joback Method
cpg	855.22	J/mol×K	889.70	Joback Method
cpg	867.97	J/mol×K	920.17	Joback Method
cpg	879.84	J/mol×K	950.65	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=U320764&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320764&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>hvac:</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>mccol:</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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