

# L-Norval, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi:	InChI=1S/C16H24N2O3/c1-4-9-14(18-16(20)21-5-2)15(19)17-12(3)13-10-7-6-8-11-13/h6
InchiKey:	ZNDAJFRHIWRDFF-JSGCOSHPSA-N
Formula:	C16H24N2O3
SMILES:	CCCC(NC(=O)OCC)C(=O)NC(C)c1ccccc1
Mol. weight [g/mol]:	292.37

## Physical Properties

Property code	Value	Unit	Source
gf	7.31	kJ/mol	Joback Method
hf	-398.04	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.779		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinsol	2147.00		NIST Webbook
tb	821.78	K	Joback Method
tc	1032.15	K	Joback Method
tf	493.91	K	Joback Method
vc	0.911	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.00	J/mol×K	821.78	Joback Method
cpg	749.47	J/mol×K	856.84	Joback Method
cpg	762.84	J/mol×K	891.90	Joback Method
cpg	775.17	J/mol×K	926.96	Joback Method
cpg	786.49	J/mol×K	962.02	Joback Method
cpg	796.84	J/mol×K	997.09	Joback Method
cpg	806.25	J/mol×K	1032.15	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=R587627&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R587627&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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