

# D-Norleu, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi:	InChI=1S/C17H26N2O3/c1-4-6-12-15(19-17(21)22-5-2)16(20)18-13(3)14-10-8-7-9-11-14
InchiKey:	CRTCXZPKJPQVGP-HIFRSBDPSA-N
Formula:	C17H26N2O3
SMILES:	CCCCC(NC(=O)OCC)C(=O)NC(C)c1ccccc1
Mol. weight [g/mol]:	306.40

## Physical Properties

Property code	Value	Unit	Source
gf	15.73	kJ/mol	Joback Method
hf	-418.68	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.169		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	844.66	K	Joback Method
tc	1054.17	K	Joback Method
tf	505.18	K	Joback Method
vc	0.968	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.26	J/mol×K	844.66	Joback Method
cpg	806.93	J/mol×K	879.58	Joback Method
cpg	820.48	J/mol×K	914.50	Joback Method
cpg	832.97	J/mol×K	949.41	Joback Method
cpg	844.43	J/mol×K	984.33	Joback Method
cpg	854.90	J/mol×K	1019.25	Joback Method
cpg	864.43	J/mol×K	1054.17	Joback Method

# Sources

<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=R587494&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R587494&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.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>

# 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>h vap:</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>r in pol:</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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