

# O-nitro carbanilic acid, 7,8-dihydrolinalyl ester

**Inchi:** InChI=1S/C17H24N2O4/c1-5-17(4,12-8-9-13(2)3)23-16(20)18-14-10-6-7-11-15(14)19(21)  
**InchiKey:** QABQBTCAMHZGAG-UHFFFAOYSA-N  
**Formula:** C17H24N2O4  
**SMILES:** C=C(C)CCCC(C)(CC)OC(=O)Nc1ccccc1[N+](=O)[O-]  
**Mol. weight [g/mol]:** 320.38

## Physical Properties

Property code	Value	Unit	Source
gf	168.19	kJ/mol	Joback Method
hf	-264.35	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.058		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
tb	891.65	K	Joback Method
tc	1120.68	K	Joback Method
tf	575.42	K	Joback Method
vc	0.992	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.72	J/molxK	891.65	Joback Method
cpg	815.50	J/molxK	929.82	Joback Method
cpg	828.22	J/molxK	967.99	Joback Method
cpg	839.97	J/molxK	1006.16	Joback Method
cpg	850.82	J/molxK	1044.33	Joback Method
cpg	860.85	J/molxK	1082.50	Joback Method
cpg	870.16	J/molxK	1120.68	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002480&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002480&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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