

# Carbanilic acid, n-nonyl ester

<b>Other names:</b>	Nonyl N-phenylcarbamate
<b>Inchi:</b>	InChI=1S/C16H25NO2/c1-2-3-4-5-6-7-11-14-19-16(18)17-15-12-9-8-10-13-15/h8-10,12-
<b>InchiKey:</b>	MEYIPBJUVYBHP5-UHFFFAOYSA-N
<b>Formula:</b>	C16H25NO2
<b>SMILES:</b>	CCCCCCCCCOC(=O)Nc1ccccc1
<b>Mol. weight [g/mol]:</b>	263.38
<b>CAS:</b>	33689-71-3

## Physical Properties

Property code	Value	Unit	Source
gf	51.72	kJ/mol	Joback Method
hf	-328.37	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	69.08	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.986		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
tb	718.62	K	Joback Method
tc	915.13	K	Joback Method
tf	327.00 ± 1.00	K	NIST Webbook
vc	0.882	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.03	J/mol×K	816.88	Joback Method
cpg	718.71	J/mol×K	849.63	Joback Method
cpg	731.50	J/mol×K	882.38	Joback Method
cpg	658.40	J/mol×K	718.62	Joback Method
cpg	674.91	J/mol×K	751.37	Joback Method
cpg	690.44	J/mol×K	784.12	Joback Method
cpg	743.44	J/mol×K	915.13	Joback Method
cps	471.10	J/mol×K	298.15	NIST Webbook

hfust	28.05	kJ/mol	327.00	NIST Webbook
hfust	28.07	kJ/mol	327.00	NIST Webbook
sfust	85.80	J/mol×K	327.00	NIST Webbook

## Sources

<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=C33689713&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33689713&amp;Units=SI</a>
<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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase 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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>sfust:</b>	Entropy of fusion at a given temperature
<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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