

# O-nitro carbanilic acid, n-octyl ester

<b>Inchi:</b>	InChI=1S/C15H22N2O4/c1-2-3-4-5-6-9-12-21-15(18)16-13-10-7-8-11-14(13)17(19)20/h7
<b>InchiKey:</b>	YOB SUUKBNXGBKX-UHFFFAOYSA-N
<b>Formula:</b>	C15H22N2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)Nc1cccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	294.35
<b>CAS:</b>	92700-70-4

## Physical Properties

Property code	Value	Unit	Source
gf	69.22	kJ/mol	Joback Method
hf	-329.96	kJ/mol	Joback Method
hfus	47.50	kJ/mol	Joback Method
hvap	84.11	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.504		Crippen Method
mvol	233.290	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	852.56	K	Joback Method
tc	1072.02	K	Joback Method
tf	566.18	K	Joback Method
vc	0.908	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.33	J/molxK	852.56	Joback Method
cpg	727.78	J/molxK	889.14	Joback Method
cpg	740.18	J/molxK	925.71	Joback Method
cpg	751.56	J/molxK	962.29	Joback Method
cpg	761.96	J/molxK	998.87	Joback Method
cpg	771.42	J/molxK	1035.44	Joback Method
cpg	779.98	J/molxK	1072.02	Joback Method

# Sources

<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>
<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=C92700704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92700704&amp;Units=SI</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>m cvol:</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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